



Calhoun: The NPS Institutional Archive
DSpace Repository

Theses and Dissertations

1. Thesis and Dissertation Collection, all items

1995

Activated carbon cloth regeneration with electrical resistance heating.

Covington, Brett A.

Monterey, California. Naval Postgraduate School

<http://hdl.handle.net/10945/25649>

Downloaded from NPS Archive: Calhoun



<http://www.nps.edu/library>

Calhoun is the Naval Postgraduate School's public access digital repository for research materials and institutional publications created by the NPS community. Calhoun is named for Professor of Mathematics Guy K. Calhoun, NPS's first appointed -- and published -- scholarly author.

Dudley Knox Library / Naval Postgraduate School
411 Dyer Road / 1 University Circle
Monterey, California USA 93943

DUDLEY LIBRARY
N. QUATE SCHOOL
MONTEREY, CA 93943-5101

**ACTIVATED CARBON CLOTH REGENERATION
with ELECTRICAL RESISTANCE HEATING**

BY

BRETT A. COVINGTON

B.M.E., Auburn University at Auburn, Alabama, 1987

INDEPENDENT STUDY

**Submitted in partial fulfillment of the requirements
for the degree of Master of Science in
Environmental Engineering in Civil Engineering
in the Graduate College of the
University of Illinois at Urbana-Champaign, 1994**

Urbana, Illinois

Thesis
C756863
C.1

ABSTRACT

Activated carbon cloth (ACC) was tested to evaluate its ability to maintain physical adsorption properties over an extended series of adsorption/desorption cycles.

Adsorption consisted of saturation with a volatile organic compound (VOC). Benzene and acetone were selected as the test VOCs due to their commonality in indoor air and potential threat to human health. Desorption of these VOCs was achieved through direct electrical resistance heating (DERH) regeneration using an alternating current to increase bulk ACC temperature to 140°C. The heat generated was due to the resistive property of the ACC's fibers (resistivity of $1-2 \cdot 10^{-2} \Omega \cdot \text{cm}$).

ACC-20 (specific surface area of 1610 m²/g and effective micropore volume of 0.636 cm³/g) was selected for this work due to its high adsorption capacity for benzene above concentrations of 200 ppmv.

The ACC-20 was tested by three similar methods. The first method involved DERH for two 6 hour periods with property evaluation after each period. The second method combined benzene saturation with DERH regeneration while the third combined acetone saturation with DERH regeneration. Both the second and the third methods were carried out for 50 adsorption/desorption cycles with property evaluation after every ten cycles.

Adsorption properties were measured by Brunauer, Emmett, and Teller (BET) nitrogen isotherms. The isotherm data were converted into specific surface area and effective micropore volume by use of the BET equation and the Dubinin Radushkevich

(DR) equation, Harkins Jura (HJ) equation, and single point method respectively. Changes in the adsorption properties of the ACC-20 were 2.2 % for BET specific surface area and 2.4 % for HJ effective micropore volume for the 12 hour DERH heated sample, 2.6 % for BET specific surface area and 3.1 % for HJ effective micropore volume for the 50 cycle benzene saturated sample, and 3.9 % for BET specific surface area and 3.8 % for single point effective micropore volume for the 50 cycle acetone saturated sample. All of these values were within the experimental error of 5.5% for BET specific surface area and 8.4 % for HJ effective micropore volume.

In addition, the purity of the VOCs was determined not degraded during the regeneration of ACC-20 by DERH.

A scaled-up estimate for an indoor air filtration system indicated that regeneration costs could be \$1450/yr for an air stream with a constant 100 ppbv benzene concentration and a flow of 57m³/min.

TABLE OF CONTENTS

Chapter

1	Introduction and Research Objective	1
1.1	Manufacture of Activated Carbon Cloth	2
1.2	Physical and Chemical Properties of Activated Carbon Cloth	2
1.3	Physical and Chemical Properties of Volatile Organic Compounds	4
2	Adsorption Theory	5
2.1	Adsorption and Desorption Isotherms	5
2.2	BET Surface Area Model	6
2.3	Micropore Volume Equations	8
2.3.1	The Dubinin-Radushkevich (DR) Equation	8
2.3.2	The Harkins Jura (HJ) statistical thickness plot	10
3	Experimental Equipment and Procedures	12
3.1	Experimental Equipment for Saturation and Regeneration	12
3.2	Experimental Procedure	12
3.2.1	Method of Saturation and Electrical Regeneration	12
3.2.2	Method of ACC Physical Characterization	14
3.2.3	Measurement of VOC Vapor Purity during Regeneration	15
3.3	Quality Control Procedures	17
4	Experimental Results and Discussion	18
4.1	Experimental Results and Sensitivity of Measurements	18
4.2	Estimation of Error in Isotherm Measurements	21
4.3	VOC Purity and Contamination Produced during Electrical Regeneration	21
4.4	Electrical Resistance and Power Requirements	21
4.5	Economical Estimation of DERH Regeneration	22
5	Conclusions and Recommendations	24
5.1	Conclusions	24
5.2	Recommendations	24
6	References	26
	Tables and Figures	28
	APPENDIX A	43

TABLES

1.1	Resistive properties of carbon fibers, metal conductors, and insulators.	29
1.2	Physical Constants of VOCs	29
4.1	Comparison of surface area and micropore volume for electrically heated ACC-20	30
4.2	Comparison of surface area and micropore volume for benzene saturated/electrically regenerated ACC-20	30
4.3	Comparison of surface area and micropore volume for acetone saturated/electrically regenerated ACC-20	31
4.4	Comparison of surface area and micropore volume from N ₂ adsorption onto untreated ACC-20, quality assurance test summary	31

FIGURES

2.1	Type I isotherm	32
3.1	Activated carbon cloth electrical regeneration apparatus	33
3.2	Rotameter calibration curve, low flow	34
3.3	Variac W10MT3 calibration	34
3.4	Variac 3PN1010 calibration	34
4.1	Nitrogen isotherm for electrically heated ACC-20	35
4.2	Nitrogen isotherm for benzene treated ACC-20	36
4.3	Nitrogen isotherm for acetone treated ACC-20	37
4.4	Dubinin-Radushkevich plot for 20 cycle acetone treated ACC-20	38
4.5	Harkins-Jura statistical thickness plot for 20 cycle acetone treated ACC-20	39
4.6	Current requirements for a 4.5 cm x 4.5 cm ACC-20 sample	40
4.7	Electrical resistance of a 4.5 cm x 4.5 cm ACC-20 sample	41
4.8	Electrical power requirements for a 4.5 cm x 4.5 cm ACC-20 sample	42

1 Introduction and Research Objectives

This research contributes to the development of a new technology for gas stream removal of volatile organic compounds (VOCs) by applying the principles of activated carbon adsorption coupled with cryogenic vapor recovery. Overall, activated carbon cloth (ACC) will be placed in a fixed bed arrangement with built in electrodes for direct electrical resistance heating (DERH) using alternating current across the ACC.

This work evaluates the effect of repetitive DERH on a single layer of activated carbon cloth attached to electrodes in a glass reactivation cell was studied. The concept of adsorption capacity regeneration by DERH first presented by Economy and Lin (1974) was extended here to evaluate the cloth's physical adsorption properties over a series of adsorption/desorption cycles. ACC was saturated with a VOC and then regenerated through DERH. The properties used to quantify the material's adsorption durability after a specific number of VOC saturation/DERH regeneration cycles were specific surface area and effective micropore volume. The power requirements to achieve complete regeneration of the sample activated carbon cloth were measured to aid in the determination of the cost effectiveness of DERH as opposed to regeneration through steam or heated gas. Furthermore, the desorbed vapor released during all regeneration was sampled to determine the purity of the VOC for recycling in an industrial process (e.g., spray paint booths, bulk fuel transfer, or part cleaning solvents).

This research is significant due to increased needs to remove indoor air contaminants, such as VOCs, because long exposure times are believed to have

serious negative health effects (Sterling, 1984 and Tancrede, 1987). Additionally, industries which emit VOCs to the atmosphere as a result of manufacturing processes will soon require new methods of control when the EPA promulgates the emission standards for the 189 hazardous air pollutants (HAPs), many of which are VOCs, listed in the Clean Air Act Amendment of 1990.

1.1 Manufacture of Activated Carbon Cloth

ACC is a cloth woven from carbon fibers then carbonized and activated through controlled oxidation heat treatment. The carbon cloth used in this research is woven from cured phenolic-aldehyde fibers made by acid-catalyzed cross-linking of melt-spun novolac resin with formaldehyde. The curing process renders the fibers both infusible and insoluble. The cloth is then carbonized and activated through a one step process in a steam or carbon dioxide atmosphere at 800° - 900°C. Surface areas produced from activation of this cloth can approach 3000 m²/g (Hayes 1981). The phenolic ACC was developed and patented by the Carborundum Company in the early 1970s through the work of Economy et al. (Hayes 1981). The final ACC material was produced and donated to perform this research by American Kynol, Inc. a subsidiary of Nippon Kynol, Inc.

1.2 Physical and Chemical Properties of Activated Carbon Cloth

A micropore is defined as having a pore width, w , less than 20 Å (Dubinin, 1960). This definition is accepted as convention by the International Union of Pure and

Applied Chemistry (Bansal, Donnet and Stockli, 1988). The pores formed during activation of the carbon cloth are hypothesized to be elongated and slit shaped with a half width between 5 and 14 Å (Economy and Lin, 1974), making these activated carbons almost entirely microporous. This is significantly different from granular activated carbon which is thought to have branched pores, with micropores mainly inside of a larger pore structure. The location of the micropores on the surface of the fibers allows for highly rapid adsorption and desorption (Hayes, 1981). This characteristic along with the structure of the woven cloth allow for *in situ* DERH at a moderate temperature of 140°C (Cal, 1993). The ACC selected for these tests was ACC-5092-20 (henceforth denoted as ACC-20). ACC-20 has a BET specific surface area of 1610 m²/g, as determined by nitrogen (N₂) adsorption at 77°C, and an effective micropore volume of 0.636 cm³/g, determined using five different reference vapors at 25°C (Foster 1992).

The electrical properties of the ACC-20 is important for the use of DERH. A moderate electrical resistance is needed to make a good resistance heater. Materials with extremely high resistances like glass or rubber will not conduct a sufficient amount of electricity for heating to occur. Conductive materials (i.e., copper and aluminum) produce very little heat due to the low resistance to current flow. In general carbon fibers (non-activated) have high resistances and in some cases can be used in insulating composite materials. However, carbon fibers may also be treated to become conductors with a resistivity as low as copper. Fibers are intercalated with alkali metals like potassium and cesium, nitric acid, and halogens through high temperature heat

treatment in a N_2 atmosphere to form highly oriented pyrolytic graphite (HOPG) within the fiber. From Table 1.1 the low resistances of pan and mesophase pitch fibers are observed after intercalation at heat treatment temperatures (HTT) (Donnet and Bansal, 1990).

Activation of carbon fibers results in a decrease in resistivity from that of cured novoloid fibers but still has a higher resistivity than the HTT fibers (Hayes, 1993). From Table 1.1 the resistivity of the fibers can be compared to typical conductors and insulators

1.3 Physical and Chemical Properties of Volatile Organic Compounds

As defined by Lewis (1989) a VOC is an organic compound with a vapor pressure, P_o , greater than 10^{-2} kPa. This is a practical definition since compounds with higher P_o values are typically found at concentrations above $0.1 \mu\text{g}/\text{m}^3$. This concentration allows for greater ease of detection than semivolatile organic compounds (SVOC) with $10^{-2} \text{ kPa} > P_o > 10^{-8} \text{ kPa}$ and concentrations in the ng/m^3 to pg/m^3 range (Nriagu, 1992). Benzene and acetone were selected as test VOCs for this research in keeping with previous work done by Fuerman (1992), Foster (1992), Cal (1993), and Graf (1994). The properties of these two VOC's which are important to this research are listed in Table 1.2.

2 Adsorption Theory

The adsorption properties of porous activated carbon have been observed since 1777 (Greg and Sing, 1982). By early this century adsorption was relatively well defined. In 1916 Langmuir published his monolayer equilibrium adsorption model and stated that charcoals were understood to be truly porous. He furthermore postulated that charcoals had cross linkage between long chain carbon molecules consisting primarily of carbon atoms. The high carbon content is a result of the majority of hydrogen and oxygen being driven off of the lignin precursor during the carbonization and activation processes.

This section discusses several methods of characterizing porous materials (specifically microporous activated carbon) which have been developed from Langmuir's time to the present day. The methods are employed in this paper to characterize ACC-20 by adsorption characteristics, and include, the adsorption isotherm, the specific surface area, and the effective micropore volume.

2.1 The Adsorption and Desorption Isotherms

Adsorption and desorption isotherms are plots of the measured number of moles (n), or volume or mass of a gas (adsorbate) adsorbed by one gram of solid material (adsorbent) as a function of the relative pressure of the adsorptive gas, P/P_0 . P is the partial pressure and P_0 is the saturation vapor pressure of the adsorbate. An adsorbent's pore size is defined by the shape of its adsorption isotherm. There are five types of isotherms as defined by the Brunauer, Deming, Deming, and Teller (BDDT)

(1940) classification. The ACC-20 used in this work was previously determined to be an almost entirely microporous solid material (Foster, 1992). For microporous solid materials the adsorption isotherm will have the characteristic shape of a Type I isotherm as found in Figure 2.1. Plotting n versus P/P_o produces an isotherm without the characteristic slightly sloping straight line at P/P_o between 0.25 and 0.95 then the material is not completely microporous.

2.2 The BET Surface Area Model

Building upon Langmuir's (1916) model for equilibrium monolayer adsorption Brunauer, Emmett, and Teller theory (BET, 1938) develops a model for multilayered adsorption. The Langmuir equation may be simplified from its original version to read:

$$\frac{v}{v_m} = \frac{BP}{1 + BP} \quad (2.1)$$

where v is the adsorption phase volume adsorbed per gram of adsorbent; v_m is the volume required to cover one gram with a monolayer of adsorbate; B is an empirical constant; and P is the partial pressure of the adsorptive. Expanding this equation through a summation of multiple layers the BET equilibrium equation is determined:

$$\frac{v}{v_m} = \frac{c(P/P_o)}{(1 - P/P_o) (1 - P/P_o + c(P/P_o))} \quad (2.2)$$

where c is typically taken to be

$$c = e^{(q_1 - q_L)/RT} \quad (2.3)$$

and q_1 is the heat of adsorption of the first layer; q_L is the heat of liquefaction for the subsequent layers; R is the ideal gas constant; and T is the absolute temperature (Brunauer, Emmett, and Teller, 1938).

To determine specific surface area using the BET model equation 2.2 is linearized.

$$\frac{1}{v \left(\left(\frac{P}{P_o} \right) - 1 \right)} = \frac{1}{v_m c} + \frac{c-1}{v_m c} \left(\frac{P}{P_o} \right) \quad (2.4)$$

After measurement of v and P/P_o from 0.01 to 0.25 (Foster, 1992) a plot is constructed from equation (2.4) of $1/[v(P/P_o - 1)]$ versus P/P_o . The slope, $(c-1)/v_m c$, and intercept, $1/v_m c$, are determined through a least squares curve fit (Greg and Sing, 1982). These values are then used to calculate v_m and c :

$$v_m = \frac{1}{\frac{1}{v_m c} + \frac{c-1}{v_m c}} \quad (2.5)$$

$$c = \frac{v_m}{\left[1 / (v_m c) \right]} \quad (2.6)$$

Now the surface area, A_{BET} is calculated using a control volume approach:

$$A_{BET} = \frac{a_m N_A v_m}{(22,414 \text{ cm}^3 (\text{STP})) (10^{20} \text{ \AA}^2/\text{m}^2)} \quad (2.7)$$

where a_m is the cross sectional area occupied by one molecule of adsorbate and N_A is Avagadros number. For nitrogen, a_m is taken to be 16.2 \AA^2 (Greg and Sing, 1982).

2.3 Micropore Volume Equations

Quantification of effective micropore volume can be characterized with several different equations applied to the N_2 adsorption isotherm data. Methods of estimating the micropore volume include the Dubinin Radushkevich (DR) equation (Dubinin, 1989), the Harkins and Jura (HJ) statistical thickness plot (Harkins and Jura, 1943, Lowell and Shields, 1984) and a single point volume adsorbed value.

2.3.1 The Dubinin Radushkevich (DR) Equation

The DR equation was developed with Dubinin's theory of the volume filling of micropores (TVFM) and is best applied as a model when using benzene or some other VOC as a reference vapor (adsorptive). Dubinin (1988) demonstrated that as a reference vapor, N_2 at 77° K is not equivalent to benzene at 293° K . Further, benzene was shown to be more appropriate for characterization of a material's adsorption properties and microporous structure. With this caveat in mind the DR equation is used only to calculate the effective micropore volume from the measured values for the volume adsorbed and the relative pressure of N_2 and is not used to model the ACC-20 adsorption characteristics for VOCs.

The DR equation is

$$W = W_o \exp \left[- \left(\frac{A}{\beta E_o} \right)^2 \right] \quad (2.8)$$

where W is the volume of the adsorbate adsorbed by one gram of the carbon; W_o is the total micropore volume available to the adsorbate; A is the differential molar work or the negative of the Gibbs free energy; β is the similarity coefficient, or the affinity factor, of the standard vapor to the reference vapor (benzene); and E_o is the characteristic adsorption energy. For N_2 , $\beta = 0.34$ (Bansal et al., 1988). The differential molar work, A , calculated as:

$$A = -\Delta G = RT \ln (P_o/P) \quad (2.9)$$

E_o is inversely related to the slit-pore half width, x_o :

$$k = x_o E_o \quad (2.10)$$

such that a constant structural factor, k , of 12.0 kJnm/mol is assumed to determine x_o (Dubinin, 1989).

The linearized DR Equation:

$$\ln (W) = \ln (W_o) - \left(\frac{1}{\beta E_o} \right)^2 A^2 \quad (2.11)$$

is used to plot $\ln(W)$ against A^2 for a range of P/P_o of 0.001 to 0.500 where W_o and x_o are determined from the slope and intercept respectively.

2.3.2 The Harkins Jura (HJ) statistical thickness plot

The concept of plotting the statistical thickness was originally proposed by Lippens and de Boer (1965) as a method of testing superposability of isotherms to standard isotherms (Lowell and Shields, 1984). Based on the so-called t-curve, a plot of the standard isotherm is produced where the statistical thickness, t , of the adsorbed film, rather than P/P_o , is the independent variable and the dependent variable is the volume adsorbed V_a . The thickness is related to the number of molecular layers, n_a/n_m (or V_a/V_m) expressed as:

$$\frac{n_a}{n_m} = \frac{V_a}{V_m} = \frac{t}{\sigma} \quad (2.12)$$

where t is the average total thickness of all layers adsorbed and σ is the thickness of one layer ($\sigma = 3.54 \text{ \AA}$ for N_2 at 77° K , assuming hexagonal close packing).

The empirical HJ equation is given as:

$$\log (P_o/P) = B + \frac{A}{V_a^2} \quad (2.13)$$

where A and B are empirical constants with A related to the thickness and the volume of a monolayer and V_a is the volume adsorbed (Harkins and Jura, 1944). This model is modified to calculate a thickness:

$$t = \left[\frac{13.99}{(0.034) - \log (P_o/P)} \right]^{1/2} \quad (2.14)$$

where 13.99 and 0.034 are empirical constants (De Boer et al., 1965). By plotting V_a against t for $P/P_o = 0.001$ to 0.7 and performing a least squares linear curve fit to the values that fit a line on the level part of the isotherm. The values selected here to best fit the Type I isotherm were for t from 0.45 to 0.70. The external surface area and micropore volume are then determined from the slope and intercept of the fitted line respectively (Micromeritics, 1987).

3 Experimental Equipment and Procedures

3.1 Experimental Equipment for Saturation and Regeneration

The intent of this experimental study is to determine the effects of repetitive heating of ACC by the application of an alternating current across the cloth to remove benzene and acetone. The effect of DERH is to be defined as any change in the adsorption properties of the cloth through changes in the micropore surface area and volume.

The experimental apparatus, Figure 3.1, centers around a glass test cell that is 40 cm long and 1.7 liters in volume with two opposing aluminum electrodes that act to support the cloth sample as well as provide electrical connections. A variable AC voltage transformer (variac), model W10MT3, provides a potential difference across the sample and current is monitored by a Fluke 77 multimeter. The bulk temperature of the cloth is monitored by a type K thermocouple detected by a digital multimeter (Omega 881C). Laboratory grade N₂ (99.95 % pure) is used to purge air and contaminants from the test cell. The exhaust gases are vented to the atmosphere via 280 lpm (10 cfm) lab venthood.

3.2 Experimental Procedure

3.2.1 Method of Saturation and Electrical Regeneration

ACCs are saturated with VOC and then regenerated through direct electrical resistance heating to complete one saturation/regeneration cycle. To determine the

durability of the cloth's adsorption properties it is necessary to run an extended number of test cycles. This section provides a detailed explanation of how this process is conducted.

ACC samples are first analyzed on a Micromeritics™ ASAP 2400 surface area analyzer, as described in section 3.2.2, to determine baseline surface areas and pore volumes prior to saturation or regeneration treatment. Prior to and between experiments ACC samples are stored in airtight bottles purged with N₂ to minimize adsorption of water vapor or contaminants.

An ACC sample is loaded into the test cell by attaching it to the electrodes and reassembling the cell. An evaporation dish containing liquid VOC (benzene or acetone) is placed into the test cell downstream of the sample. During placement the evaporation dish the cell is purged with N₂ at a minimum gas flow rate of 3 lpm. After reassembly purging is continued for a total time of 3.5 minutes. The time and flow rate for purging are estimated to provide 99.93 percent removal of air from the cell assuming that complete mixing occurs in its 1.7 liter volume. The nitrogen flow is then shutoff, the exhaust port capped and the sample is allowed to adsorb the VOC for twenty minutes at which point it is estimated that saturation is reached at room temperature (21°C). The sample is now considered saturated with VOC and the cell is prepared for DERH regeneration. Prior to DERH the evaporation dish containing the liquid VOC is removed from the test cell while purging the cell with nitrogen to prevent air from entering the test cell. During this purging it is likely that some of the VOC will desorb from the cloth as the vapor pressure in the cell is decreased by nitrogen

ventilation.

The cell is reassembled and purging continues for a total time of 3.5 minutes, then the electrical leads are attached to the electrodes with the Fluke 77 multimeter in series with the sample to measure current. N_2 flow is set at 0.5 lpm and the sample is regenerated by electrical heating at a bulk sample temperature of $140^{\circ}\text{C} \pm 10^{\circ}\text{C}$ for 20 minutes. This will require a voltage between 8 and 12 volts and a current between 0.7 and 1.1 amperes for a typical sample of 100 to 150 mg.

This procedure is repeated for ten cycles and then the ACC sample is analyzed on the ASAP 2400 to obtain measurements the specific surface area and the effective micropore volume. The samples are analyzed at 0, 10, 20, 30, and 50 cycles to measure for changes to the physical adsorption properties of the fibers in the cloth.

3.2.2 Method of ACC Physical Characterization

The Micromeritics™ ASAP 2400 surface area analyzer is a automated, multiport, N_2 BET isotherm measurement instrument. It has 12 degas stations and 6 analysis stations to allow for a high sample throughput. Analysis is controlled by an IBM AT computer with the ASAP 2400 version 3.01 software. The N_2 data measured are volume adsorbed or desorbed, partial pressure and saturation pressure. From the data the software can generate plots and calculate values for isotherms, surface area, total pore volume, and micropore surface area and volume. The calculations use the analysis methods of Langmuir (1916), BET (Brunauer, Emmett, and Teller, 1938), HJ (Harkins and Jura, 1943) and others.

To test an ACC sample it is loaded into a clean dry analysis tube (Prior to loading the sample the tube is weighed on a Mettler AE260 analytical balance with a sensitivity of 0.1 mg, to determine its mass). With the sample placed inside, the tube is loaded onto one of the degas stations. Degassing is carried out at 50 torrs absolute pressure and 140°C until desorption of gases from the sample is no longer detectable. The degas process takes between 12 and 48 hours depending on the compound adsorbed.

When the ACC has completed degassing the sample will be able to maintain a vacuum below 30 torrs with less than a 5 torrs change over a 2 minute test period. In unloading the tube is charged with N₂ before it is removed from the degas station. After cooling to room temperature the sample is reweighed on the analytical balance and the difference in mass from the tube is taken to be the ACC sample mass. Now the sample is ready for N₂ adsorption/desorption analysis.

The ASAP 2400 measures N₂ adsorption/desorption at 77.25°K (boiling point of nitrogen), this requires the dewar below the analysis station to be filled with liquid N₂. The sample tube is loaded onto the analysis port and the sample run conditions are programmed into the computer with the sample mass. After analysis the data and calculated values may be stored on electronic media for later retrieval.

3.2.3 Measurement of VOC Vapor Purity during Regeneration

To recycle a VOC desorbed from a fixed bed it is necessary to maintain VOC purity in the capture process. In this part of the experiment it is determined if the VOC, here benzene or acetone, is contaminated or altered by electrical regeneration. Equipment

used includes the glass test cell apparatus, a Hewlett-Packard gas chromatograph (GC) series HP5890, and a gas tight syringe.

Prior to testing the sample mass required to adsorb a quantity of benzene that would be detectable by the GC is calculated. By assuming that benzene behaves as an ideal gas, the ideal gas law, $PV_{\text{gas}} = nRT$, is used with $\rho = m/V_{\text{ads}}$ to write a relationship between the adsorbed volume, V_{ads} and the volume the adsorbent would occupy as a gas, V_{gas} , at some temperature, is written as:

$$\frac{V_{\text{ads}}}{V_{\text{gas}}} = \frac{PMW}{\rho RT} \quad (3.1)$$

where P is the partial pressure of the gas, MW is the molecular weight, and ρ is the density of the adsorbed benzene. The GC has a minimum detection limit of 50 ppmv so a minimum desired concentration level is arbitrarily selected at 200 ppmv. The micropore volume for the ACC-20 is 0.653 cc/g when using benzene (Foster 1992). From equation 3.1 and these two values the minimum required sample size is calculated to be 2.2 mg. Since the typical sample size used for the saturation/regeneration experiment is larger than 100 mg the GC will have no difficulty in detecting and testing benzene purity.

The sample is saturated and regenerated in the same method as described in section 3.2.1. One exception to this is no N_2 flow during regeneration. After reassembling and purging the test cell the N_2 flow is shutoff and the exhaust port is capped. Prior to regeneration a sample of the test cell gas is drawn with a gas tight syringe. Analysis of the gas sample with the GC determines initial VOC concentration.

During regeneration the test cell gas is sampled at two minute intervals and analyzed to determine VOC concentration and composition.

3.3 Quality Control Procedures

The rotameter used to determine the purge nitrogen gas flow rate was calibrated by using a 1000 ml bubble meter. The calibration curve produced by the bubble meter is linear by least squares curve fit (Figure 3.2). This linear relationship is used to convert the rotameter values into liters per minute (lpm) of gas flow.

The variac voltage was calibrated by using a separate sample in the test cell and the Fluke 77 multimeter in parallel with the sample circuit. Test voltages on the variac ranged between 0 and 15 volts. This range provided sufficient heating for a typical sample of 100 to 150 mg. The calibration curve for the W10MT3 variac, General Radio Co. is shown in Figure 3.3 is utilized to adjust the voltage given by the variac to the actual voltage. The 3PN1010 variac was used on a few of the acetone regeneration cycles, the calibration curve for this variac is given in Figure 3.4.

4 Experimental Results and Discussion

This section provides the experimentally determined values which characterize the ACC-20 as it is exposed to numerous adsorption/desorption cycles through VOC saturation followed by DERH. Those values include the BET specific surface area, DR, HJ and single point effective micropore volumes. All values are calculated from the BET adsorption isotherm with N_2 as the standard vapor. Error experienced in analyzing was determined by repetitive testing of a single sample without cyclical treatment or DERH.

4.1 Experimental Results

The ASAP 2400 recorded N_2 adsorbed and desorbed at relative pressure from 0.001 to 1.0 to produce the adsorption and desorption isotherms. Three ACC-20 samples were analyzed on the ASAP 2400. Each sample was initially analyzed to establish baseline values for the specific surface area and effective micropore volumes. The first sample did not undergo VOC saturation. The ACC-20 was heated by DERH for two six hour periods with analysis after each period. The second sample of ACC-20 was cycled by saturation with benzene and regeneration by DERH. The third sample of ACC-20 was cycled by saturation with acetone and regeneration by DERH. Both the second and third samples were subjected to 50 adsorption/desorption cycles with analysis after every 10 cycles.

The N_2 adsorption and desorption isotherms in Figures 4.1 to 4.3 are standard Type I isotherms and clearly define this ACC-20 as microporous (Greg and Sing,

1985). The variation between the isotherms produced before treatment and those produced after exposure to an alternating current (AC) is less than 7 %. The AC power is supplied at 1.67 amps and 11 volts to heat the sample at 140°C for periods of 6 hours . Figure 4.2 and Figure 4.3 for benzene and acetone cycled ACC-20 respectively indicate similar results to the electrically heated ACC-20. Each figure shows the adsorption and desorption isotherms for the baseline and after samples were exposed to 50 saturation/regeneration cycles. A slight increase in the volume adsorbed at 12 hours and 50 cycles may be noted in these figures. However, the increase is small and below a measurable significance.

The DR effective micropore volume was determined by a plot of the natural logarithm of N_2 volume adsorbed, $\ln(W)$, against the square of the differential molar work, A^2 , calculated from the measured relative pressure of N_2 . As seen in Figure 4.4, the isotherm data for the 20 cycle acetone treatment is graphed on a DR plot. A least squares linear curve fit provides a value of -0.0220 for $\ln(W_0)$, which results in a W_0 of 389.9 cm^3/g for the adsorption capacity of N_2 gas or an effective micropore volume of 0.6031 cm^3/g .

As an alternative method of calculating the micropore volume a HJ statistical thickness plot (t-plot) is generated. Figure 4.5 provides a t-plot of 20 cycle acetone saturation/DERH regeneration and indicates the volume of N_2 gas adsorbed is 366.15 cm^3/g or a effective micropore volume 0.566 cm^3/g . Also, the single point effective micropore volume is measured at a P/P_0 of 0.95. For a completely microporous material like the ACC the values measured are close to those calculated with the DR

and HJ equations. Tables A.1 to A.13 provide the data measured and results calculated in determining the micropore volumes for each 6 hour heat treatment or 10 cycle sample.

When the ACC-20 is heated to 140°C for extended times using DERH the material does not show any appreciable change in specific surface area or effective micropore volume. Table 4.1 compares these properties after 0, 6, & 12 hours of heating time. The percent difference (Δ %) is taken as the change from the properties found at the 0 hour as a baseline. The ACC-20 sample is shown to have increased in BET specific surface area by only 2.2 % while the largest effective micropore volume increase is seen by the HJ equation at 2.4 %.

Table 4.2 gives calculated adsorption values for the 0 to 50 cycles of benzene saturation with DERH regeneration. A 40 cycle analysis was not performed due to the lack of significant change between 0 and 30 cycles. Samples were not cycled beyond 50 cycles due to the manual effort and time required in each saturation/regeneration cycle and a three day per sample BET analysis period.

The combination of benzene saturation with DERH regeneration is shown not to significantly effect the adsorption capacity of the ACC-20 as determined by its affinity for N₂ adsorption at 77.25°K. The largest changes are an increase in the BET specific surface area by 7.7 % and the HJ effective micropore volume by 8.49 %, which occur after 20 cycles. This variation is considered small when compared to error values of more than 10 % reported by Dubinin (1989) and Cal (1993). Likewise the cycles of acetone saturation with DERH regeneration have similar results with surface area

increasing by 3.9 % and single point effective micropore volume increasing by 3.8 % as listed in Table 4.3.

4.2 Estimation of Error in Isotherm Measurements

To determine the accuracy provided by the ASAP 2400 when measuring the microporous ACC-20 samples, a clean unused ACC sample was tested three times sequentially to check for the repeatability of measured results. An average value and standard deviation were calculated along with each runs variation from the initial value and is provided in Figure 4.4. This sample was found to have the highest variation with an 8.4 % increase of the HJ effective micropore volume in the third test.

4.3 VOC Purity and Contamination Produced during Electrical Regeneration

The 123.5 mg ACC-20 sample used for the benzene cycle test was regenerated and then saturated with benzene. In the next regeneration gas samples (10 cm³ each) were drawn out of the test cell and injected into the GC as outlined in section 3.2.3. A single peak for benzene was produced with a concentration near 5% by volume and no impurities were found. A similar experiment on the 131 mg ACC-20 acetone sample produce a single peak for acetone with no impurities found.

4.4 Electrical Resistance and Power Requirement

The electrical current and voltage were measured over a temperature range of 23° to 300°C for a 4.5 cm x 4.5 cm square sample of ACC-20 oriented with the cloths

primary weave in the direction of current flow. Figure 4.6 shows the relation between current and temperature which was determined to be linear over this temperature range. Using ohms law the resistance of the ACC-20, plotted as a function of temperature in figure 4.7, was found to have an asymptotic decline from 50° to 270°C. However, it is not understood why the resistance briefly increases before reaching 50°C. This decrease in resistance of the bulk cloth over increasing temperatures is similar to the decrease in resistivity found on pristine PAN and pitch fibers by Lee, et al. (Donnet and Bansal, 1990).

The power required to achieve heating of the cloth was calculated from the measured values of the root mean square voltage, V_{RMS} , and current, I_{RMS} , with the assumption that the phase angle, θ , between the voltage and the current was 0° (Power = $V_{RMS} I_{RMS} \cos \theta$). Thereby a worst case estimation of power consumed is provided. The power requirements in Figure 4.8 indicate a linear relationship to temperature when a single sheet of ACC-20 is heated by DERH..

4.5 Economical Estimation of DERH Regeneration

Using the power requirements calculated for the 4.5 cm X 4.5 cm square sample of ACC-20, Graf's (1994) filter mass requirements of 1.36 Kg for ACC-10 in a full-scale filtration estimate for 57 m³/min (2,000 cfm) indoor air ventilation and a 2/1 relationship of low concentration adsorption capacities between ACC-10 and ACC-20 (Foster, 1992) an estimation of energy costs is made for a full-scale filtration system. The energy required per regeneration is calculated from a constant power requirement of 35

W over an estimated 30 minutes for a 400 mg sample. By assuming an energy price of \$0.08/kWhr and a regeneration interval of 2.4 days the energy cost would be \$1450/year. This cost seems to be slightly high considering that a ventilation rate of 57 m³/min (2,000 cfm) will only provide ten air changes per hour to a 223 m² (2,400 ft²) building

It is important to notice that this is strictly the cost to heat the filter and does not include the cost for preheating N₂, or energy to run additional fans and damper motors. This cost could vary significantly for a fixed bed when taking into account the possibility of increased conductance due to bed configuration, nonlinear power/temperature relationships or the cooling effect of a N₂ flow through the ACC. Further, the power requirement was based on heating the ACC-20 while suspended in a glass test cell surrounded by 1.7 liters of N₂ gas. Therefore, it is anticipated that convection heat transfer in the cell was significant and that the power requirements to produce the same temperatures in a fixed bed with preheated nitrogen flow could be substantially lower.

5 Conclusions and Recommendations

5.1 Conclusions

The activated carbon cloth (ACC-20) displays a high level of durability by maintaining adsorption characteristics at relatively constant values for up to 50 adsorption/desorption cycles, with VOC adsorbate saturation and direct electrical resistance heating (DERH) regeneration at a temperature of $140 \pm 10^{\circ}\text{C}$. The BET specific surface area and effective micropore volume remain within 8 % of the baseline values measured before cyclic testing. The DERH current and power requirements for suspended sheet ACC-20 have increasing linear relationships with the desorption temperature, while the bulk sample resistance decreases with increasing desorption temperatures above 60°C . Scaled up estimations of power requirements and energy costs indicate that DERH could be costly for removal of low concentration VOCs in an indoor air environment when the VOC concentration is a constant 100 ppbv of benzene, regeneration is required every 2.4 days, and there are 10 air changes per hour. The benzene and acetone adsorbed by the ACC-20 were tested for purity during regeneration by DERH. It was determined that these two VOCs do not breakdown and are not contaminated by the carbon cloth.

5.2 Recommendations

Quantifying the ACC-20 adsorption characteristics by measurement of the effective micropore volume would be more appropriately determined by using the actual test

VOC or an approved reference vapor (benzene) in a total gas analyzer or a gravimetric balance apparatus (Cal, 1993). This will allow the Dubinin-Radushkevich equation to be applied as a model to various VOCs using affinity coefficients, β . Additionally this would be a better determination of the ACC's ability to regain an original adsorption capacity for the particular contaminant.

Kinetic studies of regeneration times and power requirements should be performed on a pilot scale fixed bed adsorption system to accurately determine the feasibility and economics of applying DERH as the method of *in situ* regeneration as opposed to regeneration by heated gas or steam.

Stability and purity measurements for other VOCs (acetaldehyde, methylethyl ketone, toluene, etc.), found in indoor and industrial air streams, need to be made to determine wide spread application of this regeneration method.

6.0 References

- Avallone, E.A. and Baumeister, T., *Marks' Standard Handbook for Mechanical Engineers*, McGraw-Hill, Inc. New York, 1987, 15-1 to 15-29
- Bansal, R.C., Donnet, J-B., and Stockli, F., *Active Carbon*, Marcel Dekker, Inc., New York, 1988
- Brunauer, S., Emmett, P.H., and Teller, E., *J.Amer. Chem. Soc.*, **60**, 1938, 309
- Brunauer, S., Deming, L.S., Deming, W.S., and Teller, E., *J.Amer. Chem. Soc.*, **62**, 1940, 1723
- Cal, M.P., *Adsorption and Experimental Verification of the Adsorption of Volatile Organic Compounds onto Activated Carbon Fibers*, Master's Thesis, Univ. of Illinois-Urbana, 1993
- de Boer, J.H et al., *J. of Colloid and Interface Sci.* **21**, 1966, 415-434
- Donnet, J-B. and Bansal, R.C., *Carbon Fibers*, 2nd ed, Marcel Dekker, Inc., New York, 1990
- Dubinina, M.M., *Zhur. Phys. Chem.* 34, 1960, 959 ; *Chem Rev.* **60**, 1960, 235
- Dubinina, M.M., *Carbon*, **27**, no.3 1989, 457-467
- Dubinina, M.M., Polyakov, N.S., and Kataeva, L.I. *Carbon*, **29**, nos.4/5 1991, 481-488
- Economy, J. and Lin R.Y., *J. Mater. Sci.* **6**, 1971, 1151
- Economy, J. and Lin R.Y., *Appl. Polymer Symp.* **29**, 1976, 199-211
- Fuerman, B.G., *Adsorption of Indoor Organic Gases Onto Activated Carbon Fibers*, Master's Theses, Univ. of Illinois-Urbana, 1992
- Graf, O. W., *Analysis of Breakthrough Times of Volatile Organic Compounds for Activated Carbon Fibers in Packed Beds*, Master's Thesis, Univ. of Illinois-Urbana, 1994
- Gregg, S.J., Sing, K.S.W., *Adsorption, Surface Area and Porosity*, 2nd ed., Academic Press, London, 1982
- Hayes, J.S., *Kirk-Othmer: Encyclopedia of Chemical Technology*, 16, 3rd ed, 1981,

125-138

Hayes, J.S., *Direct communication with American Kynol Inc.*, April, 20 1993

Langmuir, I.J., *Amer. Chem. Soc.* **38**, 1916, 2221

Lewis, R. G., *J. Chin. Chem. Soc.* **36**, 1989, 261-277

Lide, D. R., Ed. *Handbook of Chemistry and Physics*, 73 ed.; CRC, Boca Raton, 1993

Lin R.Y. and Economy, J., *Appl. Polymer Symp.* **21**, 1973, 143

Lowell, S. and Shields, *Powder Surface area and Porosity*, Chapman and Hall, London 1984

Nrigau, J.O., Ed. *Gaseous Pollutants, Characterization and Cycling*, John Wiley & Sons, Inc., New York, 1992, 338-339

Sterling, D. A., *Indoor Air and Human Health*, Proceedings of the 7th Life Sciences Symposium, Knoxville, TN, 1984

Tancrede, M., Wilson R., Zeise L., Crouch E.A., *Atmospheric Environment*, **21**, no. 10, 1987, 2187-2205

Tables and Figures

Table 1.1 Resistive properties of carbon fibers, metal conductors, and insulators

Phenolic Based Carbon Fibers^a	Resistivity (Ω-cm)	Conducting Metals^c	Resistivity ($\mu\Omega$-cm)
cured novolac	10^{15} - 10^{16}	copper	1.724
carbon HTT @ 800°C	1 - 3×10^{-4}	aluminum	2.828
carbon HTT @ 2000°C	1 - 2×10^{-4}	iron wire	97.8
ACC (1500m ² /g)	1 - 2×10^{-2}		
ACC (2000m ² /g)	1 - 3×10^{-3}		
Other HTT Carbon Fibers^b	Resistivity ($\mu\Omega$-cm)	Insulating Materials^c	Resistivity (MΩ-cm)
PAN	830	Bakelite	5 - 30×10^{11}
mesophase pitch	400	glass	17×10^9
vapor grown	77	polyvinyl chloride	10^{11} - 10^{15}

a. Hayes (1993), b. Donnet and Bansal (1990), c. Avallone and Baumeister (1987)

Table 1.2 Physical properties of VOCs (Lide 1993)

Compound	Molecular weight (g/gmol)	Boiling Point (°C)	Liquid Density at 298°K (g/cm³)	Vapor Pressure at 298°K (kPa)
benzene	78.11	80.1	0.8765	12.77
acetone	58.06	56.2	0.7899	30.61

Table 4.1 Comparison of surface area and micropore volume for electrically treated ACC-20

Number of cycles	Sample Mass (mg)	BET Surface area (m ² /g)	% dif	DR micropore volume (cc/g)	% dif	HJ micropore volume (cc/g)	% dif	single point micropore volume (cc/g)	% dif
0	129.1	1319.5	0.0%	0.6166	0.0%	0.5795	0.0%	0.6234	0.0%
6	127.4	1304.2	1.2%	0.6088	1.3%	0.5733	1.1%	0.6157	1.2%
12	120.3	1349.0	2.2%	0.6265	1.6%	0.5931	2.4%	0.6374	2.3%

Table 4.2 Comparison of surface area and micropore volume for benzene treated ACC-20

Number of cycles	Sample Mass (mg)	BET Surface area (m ² /g)	% dif	DR micropore volume (cc/g)	% dif	HJ micropore volume (cc/g)	% dif	single point micropore volume (cc/g)	% dif
0	133	1309.2	0.0%	0.6121	0.0%	0.5744	0.0%	0.6202	0.0%
10	131.4	1404.9	7.3%	0.6558	7.1%	0.6223	8.3%	0.6587	6.2%
20	125.2	1409.4	7.7%	0.6574	7.4%	0.6228	8.4%	0.6635	7.0%
30	122.8	1310.5	0.1%	0.6115	0.1%	0.5777	0.6%	0.6149	0.9%
50	123.5	1343.4	2.6%	0.6254	2.2%	0.5923	3.1%	0.6326	2.0%

Table 4.3 Comparison of surface area and micropore volume for acetone treated ACC-20

Number of cycles	Sample Mass (mg)	BET Surface area (m ² /g)	% dif	DR micropore volume (cc/g)	% dif	HJ micropore volume (cc/g)	% dif	single point micropore volume (cc/g)	% dif
0	140.4	1298.6	0.0%	0.6078	0.0%	0.5726	0.0%	0.6140	0.0%
10	133.5	1312.2	1.0%	0.6121	0.7%	0.5800	1.3%	0.6146	0.1%
20	134.7	1290.2	0.6%	0.6031	0.8%	0.5664	1.1%	0.6084	0.9%
30	131.4	1319.3	1.6%	0.6168	1.5%	0.5770	0.8%	0.6140	0.0%
50	131.1	1349.0	3.9%	0.6265	3.1%	0.5916	3.3%	0.6374	3.8%

Table 4.4. Comparison of surface area and micropore volume from N₂ adsorption onto untreated ACC-20, quality assurance test summary

QA test sample	Sample Mass (mg)	BET Surface area (m ² /g)	% dif	DR micropore volume (cc/g)	% dif	HJ micropore volume (cc/g)	% dif	single point micropore volume (cc/g)	% dif
1	84.7	1201.8	0.0%	0.6121	0.0%	0.5744	0.0%	0.6202	0.0%
2	106.9	1231.8	2.5%	0.6558	7.1%	0.6223	8.3%	0.6587	6.2%
3	108.2	1136.2	5.5%	0.6574	7.4%	0.6228	8.4%	0.6635	7.0%
average		1189.9		0.6418		0.6065		0.6475	
std. deviation		39.9		0.0210		0.0227		0.0194	

Figure 2.1 Type I isotherm

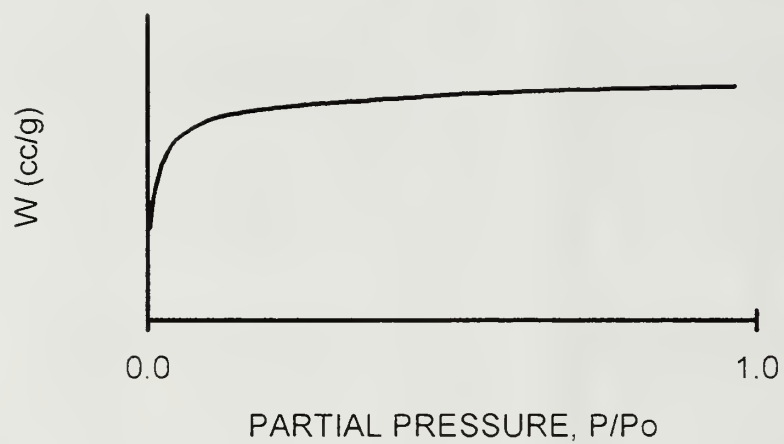


Figure 3.1 Activated carbon cloth electrical regeneration apparatus

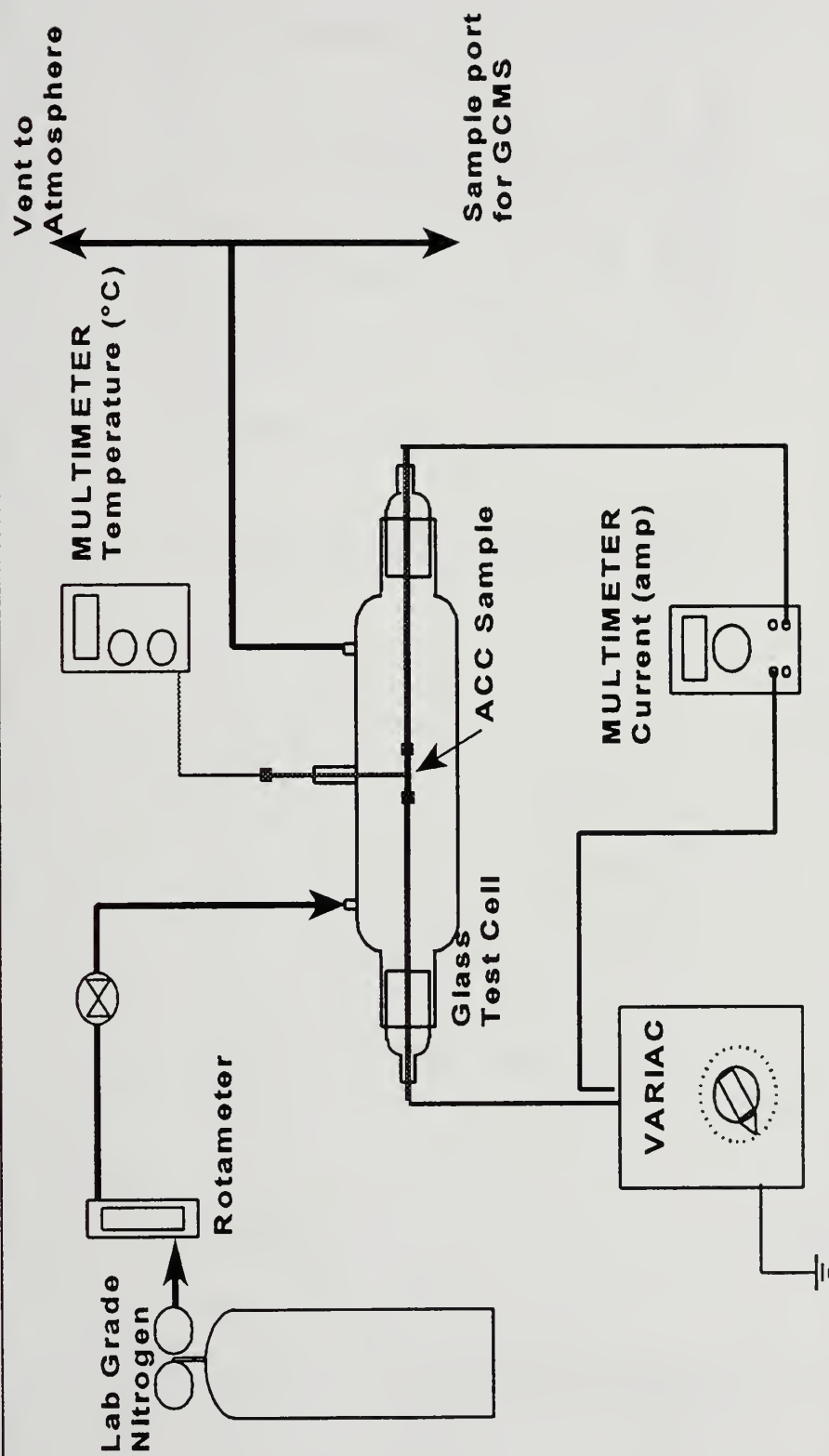


Figure 3.2 Rotometer calibration curve, low flow

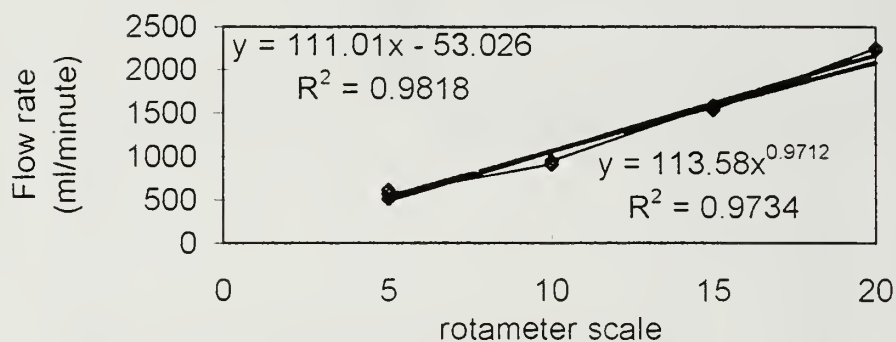


Figure 3.3 Variac W10MT3 Calibration

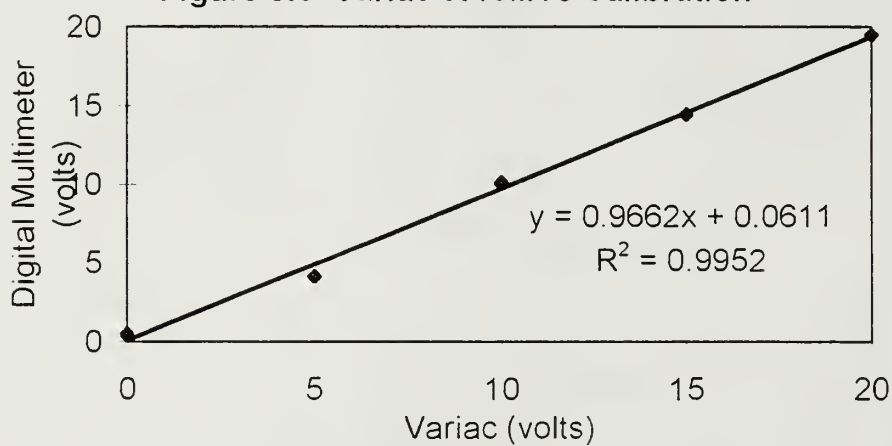


Figure 3.4 Variac 3PN1010 Calibration

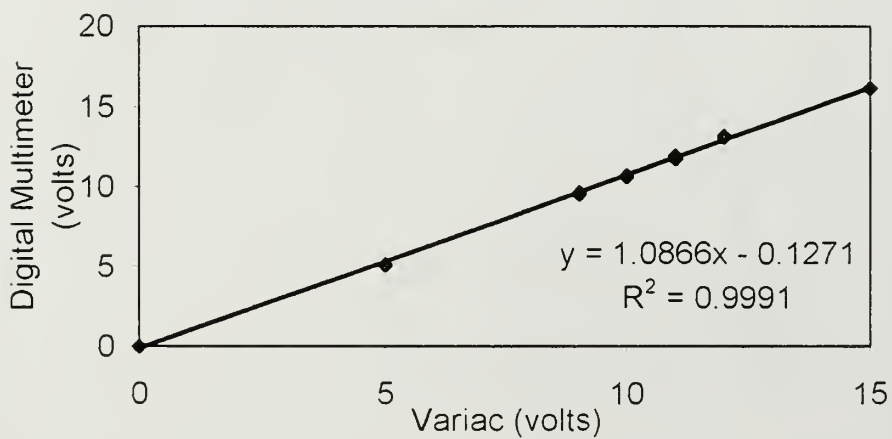


Figure 4.1 Nitrogen isotherm for electrically heated ACC-20

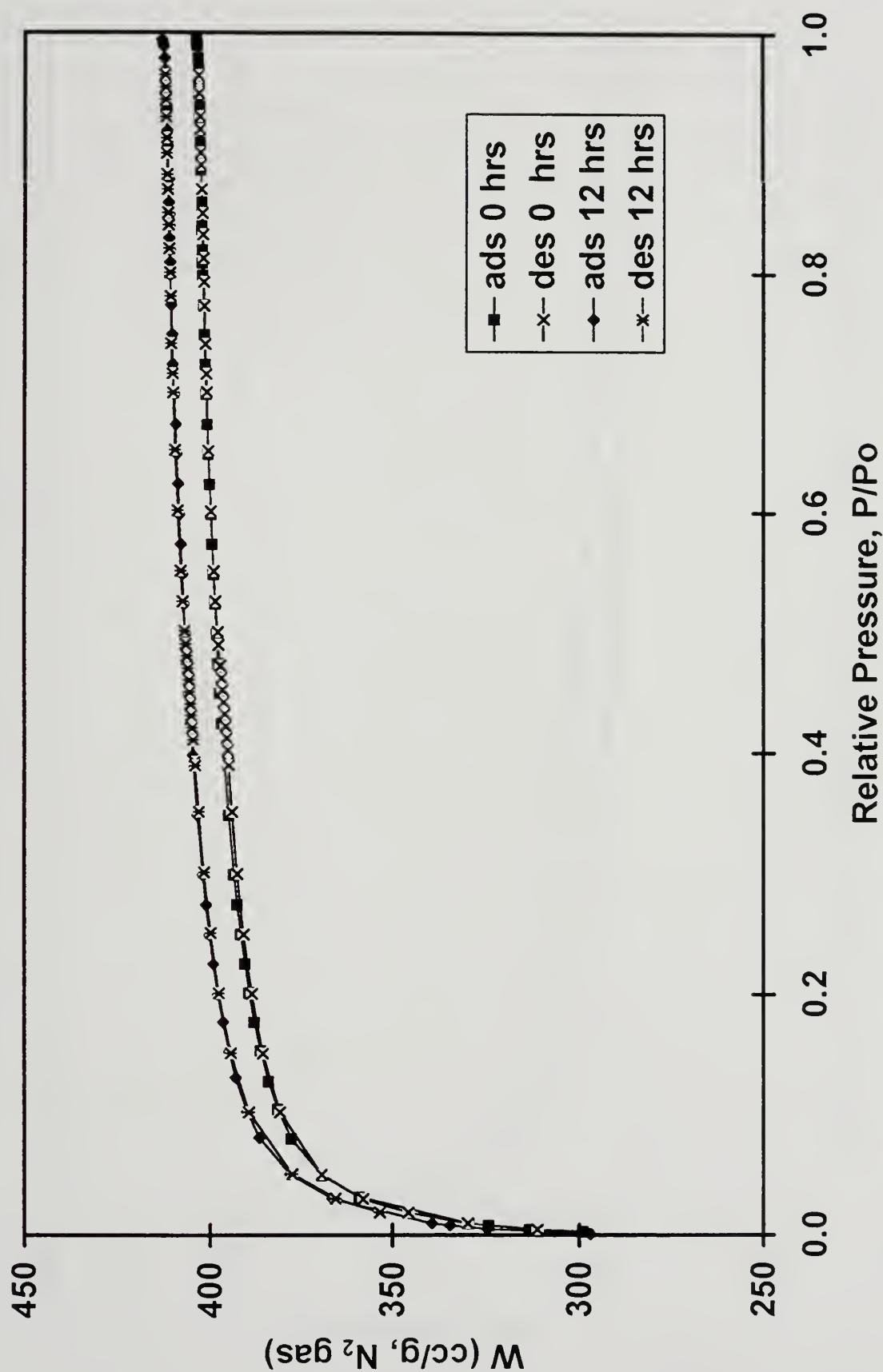


Figure 4.2 Nitrogen isotherms for benzene treated ACC-20

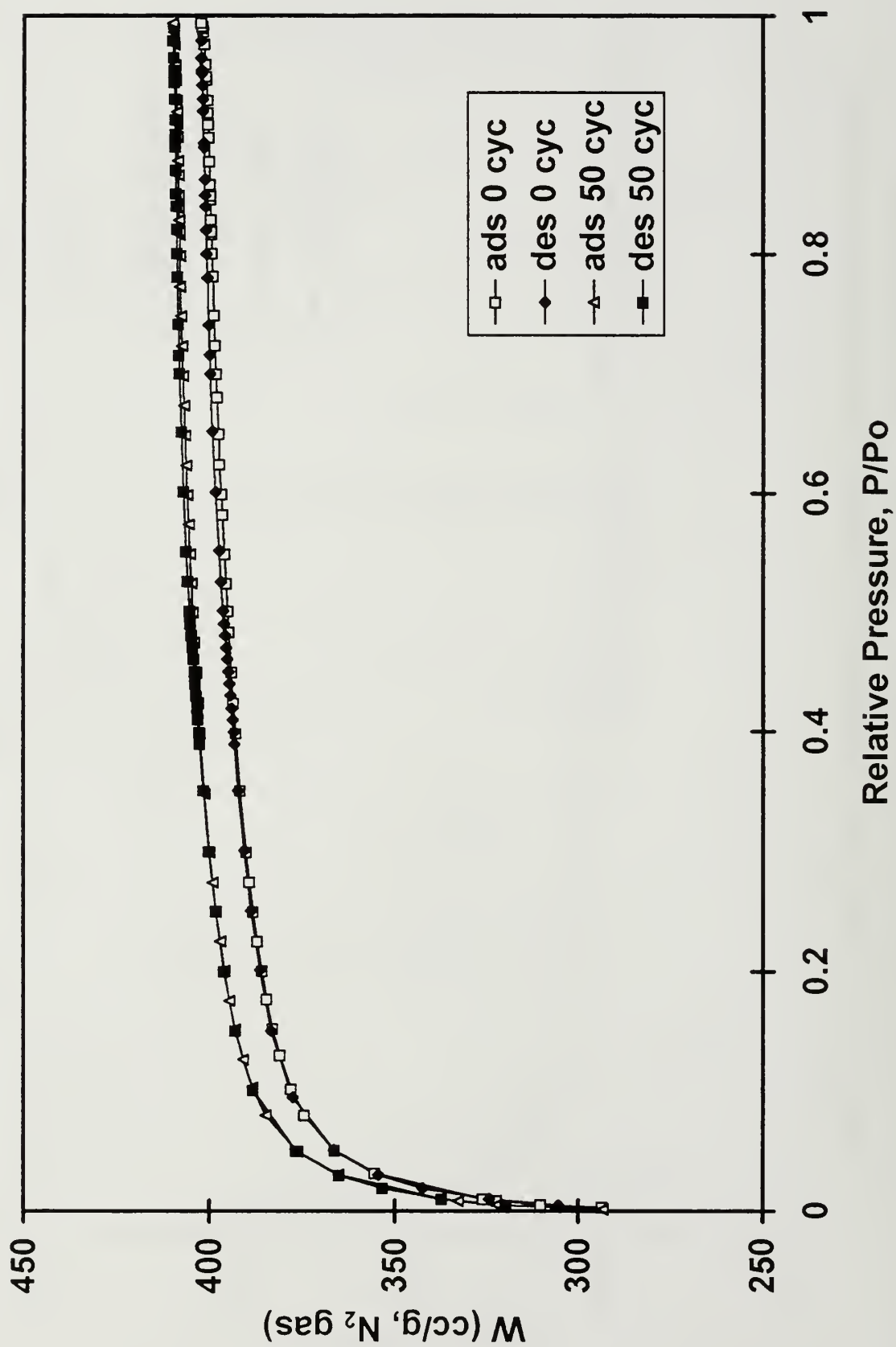


Figure 4.3 Nitrogen isotherms for acetone treated ACC-20

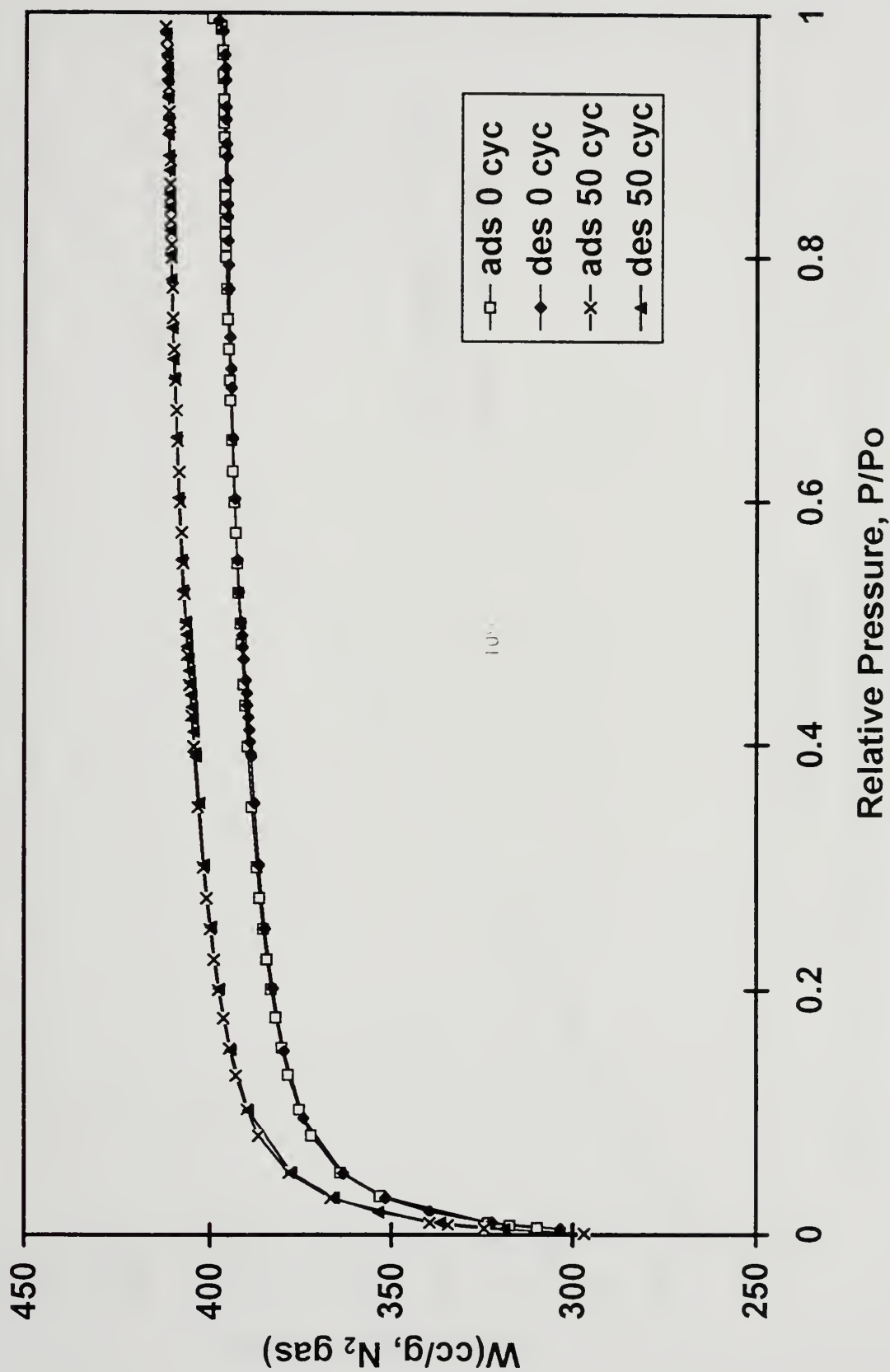


Figure 4.4 Dubinin-Radushkevich plot for 20 cycle acetone treated ACC-20

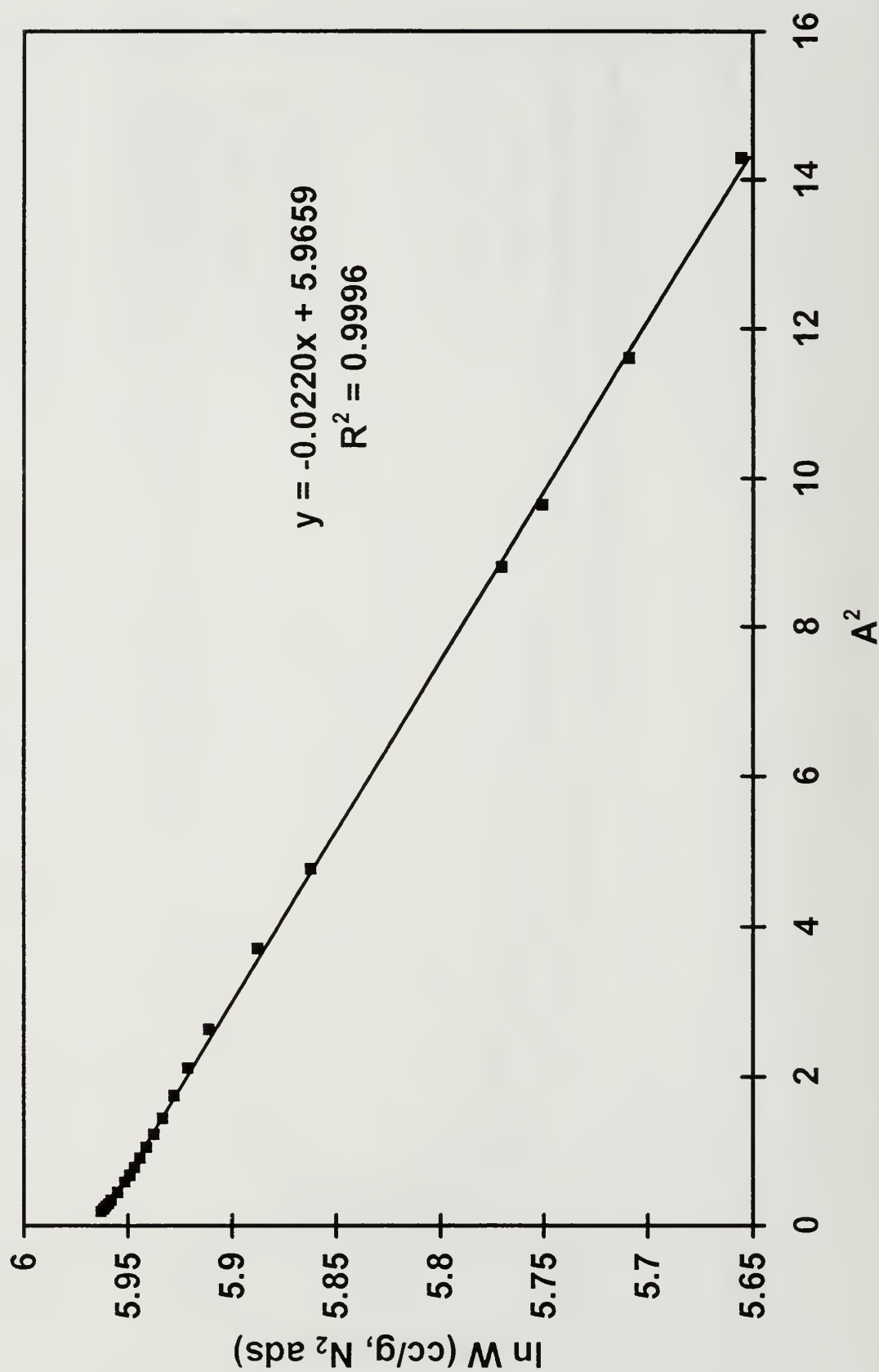


Figure 4.5 Harkins-Jura statistical thickness plot for 20 cycle
acetone treated ACC-20

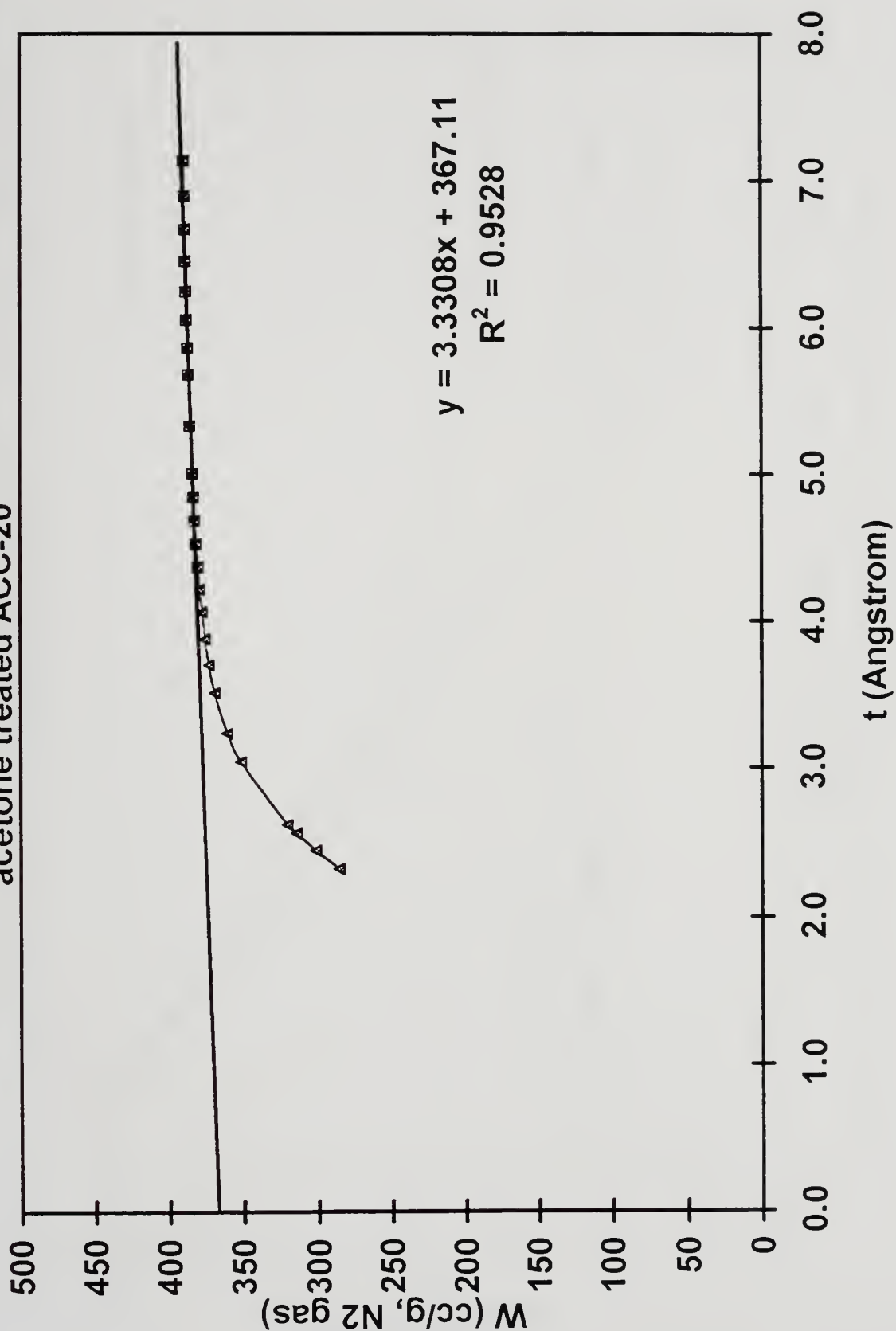


Figure 4.6 Current requirements for a 4.5 cm x 4.5 cm
ACC-20 sample

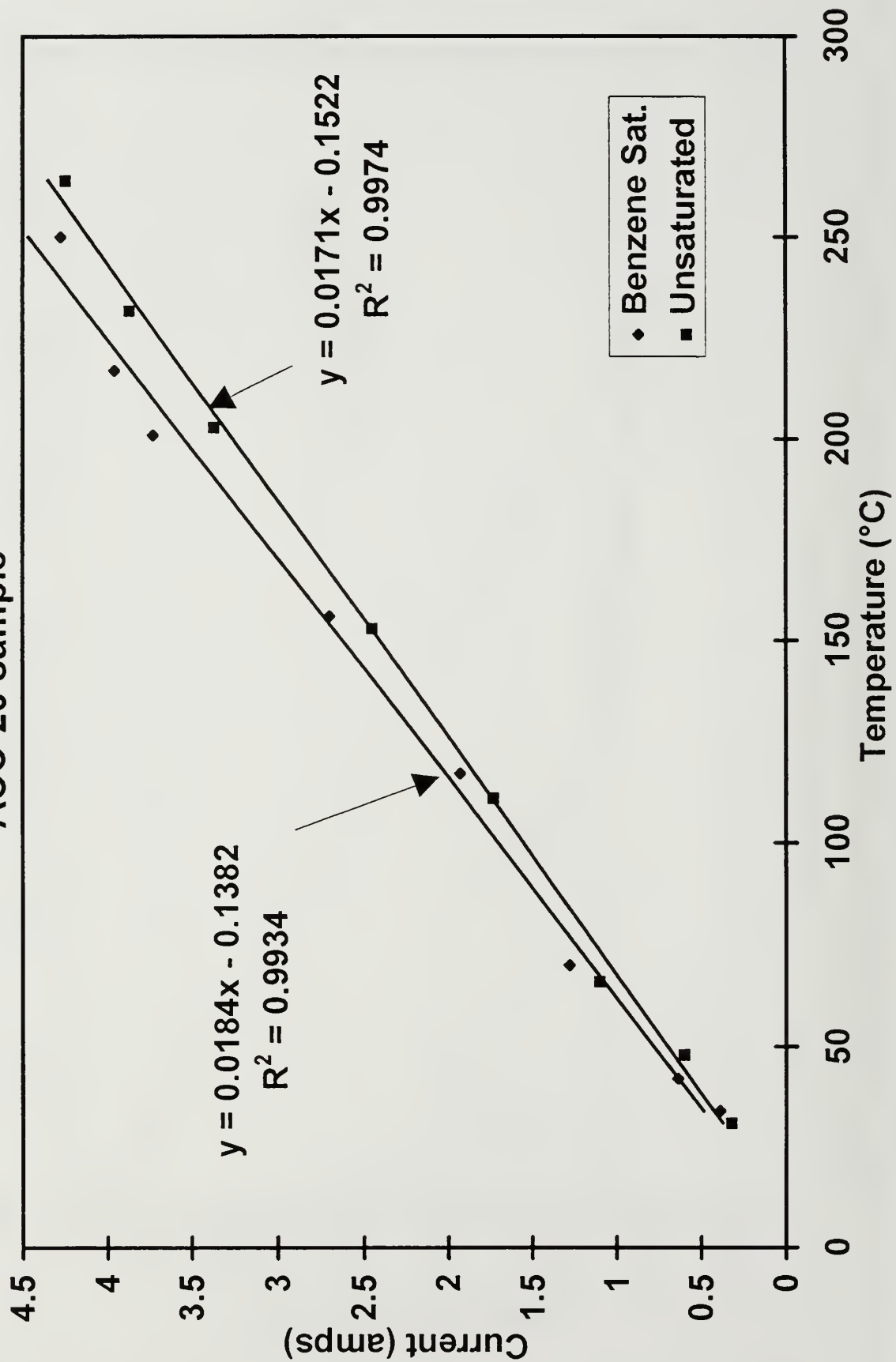


Figure 4.7 Electrical resistance of a 4.5 cm x 4.5 cm
ACC-20 sample

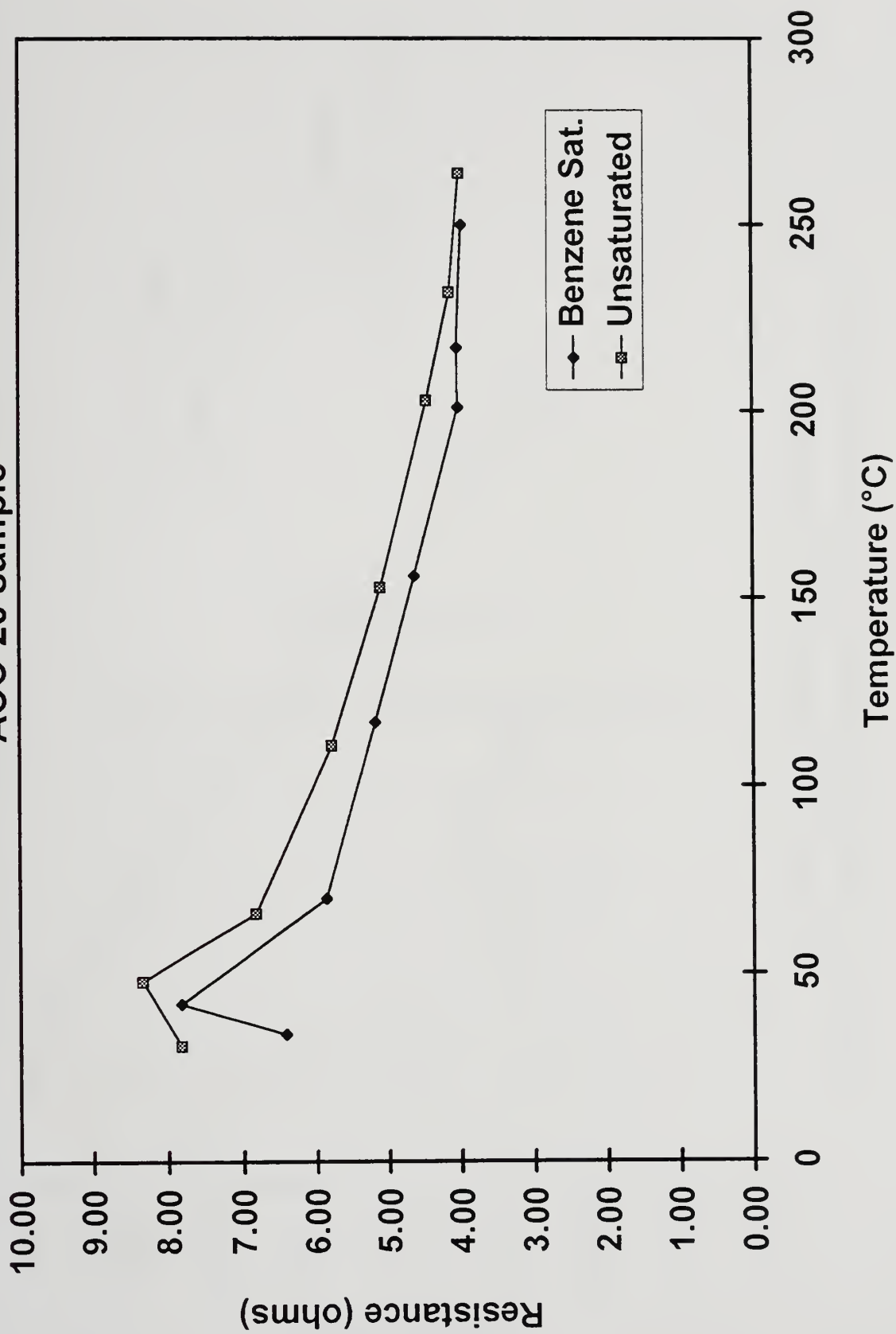
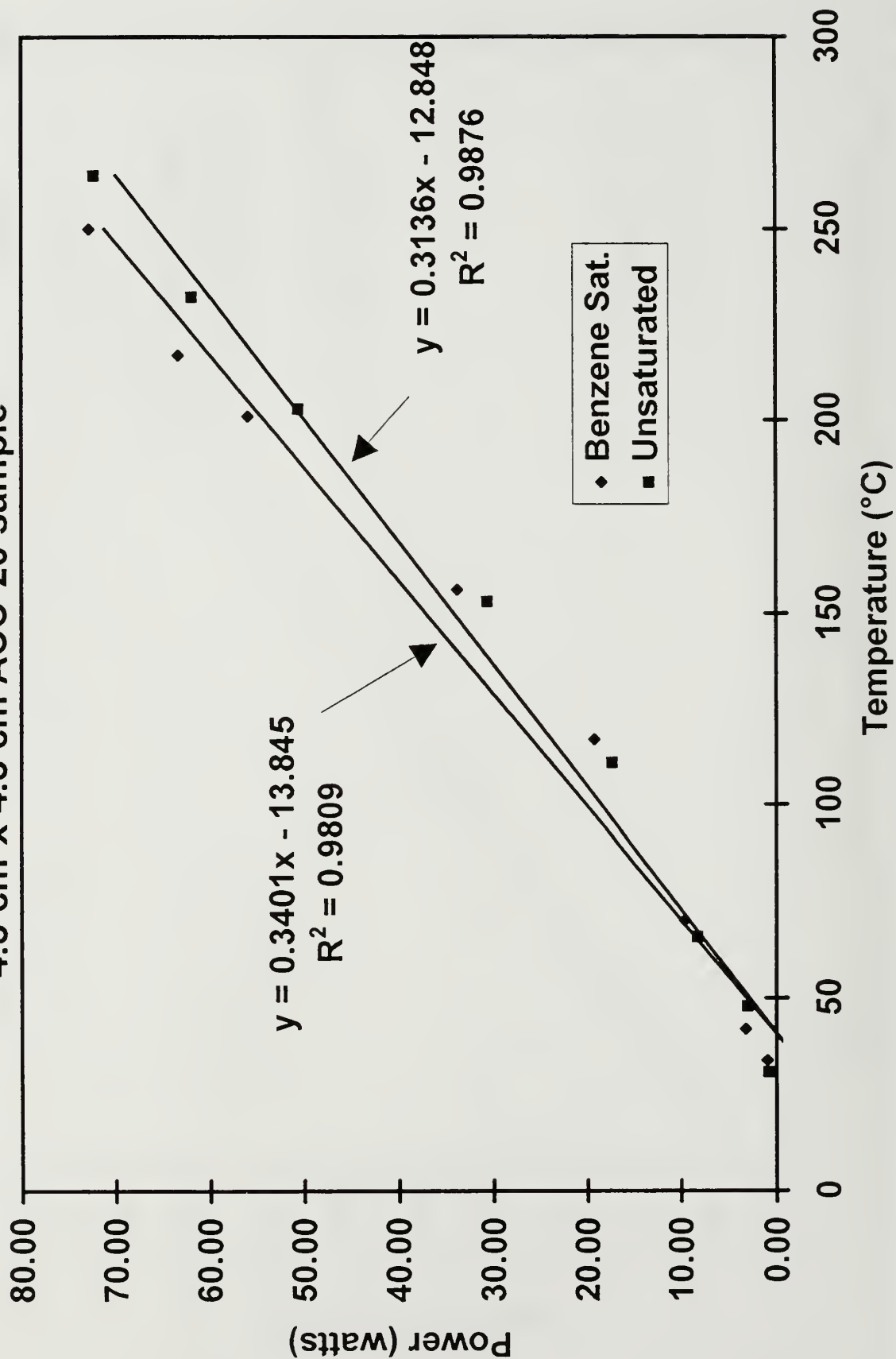


Figure 4.8 Electrical power requirements for a
4.5 cm x 4.5 cm ACC-20 sample



APPENDIX A

Experimental Data and Calculations

Table A .1. Micropore volume calculations from N₂ adsorption onto ACC-20, baseline heating

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t(Angstrom)	
0.0029	298.9251	14.1195	5.7002		K 12.0000 kJ-nm/g-mole
0.0049	312.8724	11.6983	5.7458		β 0.3400
0.0079	323.9587	9.6915	5.7806		T 77.3500 ° K
0.0099	329.3827	8.8090	5.7972		R 0.0083 kJ/g-mole-K
0.0314	358.8644	4.9537	5.8829		n 2.0000
0.0497	369.4262	3.7264	5.9120		C(ads/gas) 646.4962
0.0801	378.0094	2.6356	5.9349		
0.1043	381.6808	2.1132	5.9446		
0.1274	384.1987	1.7557	5.9512		D-R equation results
0.1531	386.327	1.4565	5.9567		slope -0.0209 (kJ/mol) ²
0.1771	387.9185	1.2392	5.9608		intersept 5.9881 (kJ/mol) ²
0.2013	389.337	1.0626	5.9644	4.3772	R ² 0.9989
0.2254	390.5075	0.9180	5.9674	4.5323	R 0.9995
0.2502	391.5883	0.7939	5.9702	4.6911	W ₀ 398.6369 cc/g (N ₂ gas)
0.275	392.5487	0.6893	5.9727	4.8503	W ₀ (ads) 0.6166 cc/g (N ₂ ads)
0.2999	393.4418	0.5998	5.9749	5.0116	E ₀ 20.3631 kJ/mol
0.3484	394.8575	0.4598	5.9785	5.3329	x 0.5893 nm
0.3983	396.095	0.3505	5.9817	5.6790	
0.4237	396.7072	0.3050	5.9832	5.8633	H-J equation results
0.449	397.2421	0.2652	5.9845	6.0536	slope 3.6484 cc/gA
0.4738	397.6791	0.2308	5.9856	6.2477	intersept 374.6301 cc/g (N ₂ gas)
0.4984	398.156	0.2005	5.9868	6.4486	R ² 0.9531
0.5238	398.5717			6.6660	R 0.9763
0.5736	399.3608			7.1274	W ₀ 374.6301 cc/g (N ₂ gas)
					W ₀ (ads) 0.5795 cc/g (N ₂ ads)
0.9491	403.0132				Single Point
					W ₀ (ads) 0.6234 cc/g (N ₂ ads)

Table A .2. Micropore volume calculations from N₂ adsorption onto ACC-20, 6 hours heating

P/P _o	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)		
0.0029	294.7783	14.1195	5.6862		K	12.0000 kJ-nm/g-mole
0.0052	309.3126	11.4383	5.7344		β	0.3400
0.0082	320.3971	9.5429	5.7696		T	77.3500 ° K
0.0099	324.8708	8.8090	5.7834		R	0.0083 kJ/g-mole-K
0.0308	353.6885	5.0091	5.8684		n	2.0000
0.0492	364.3482	3.7515	5.8981		C(ads/gas)	646.4962
0.0799	373.0650	2.6409	5.9218		D-R equation results	
0.1036	376.6842	2.1258	5.9314			
0.1269	379.2552	1.7624	5.9382		slope	-0.0210 (kJ/mol) ²
0.1525	381.3820	1.4626	5.9438		intersept	5.9753 (kJ/mol) ²
0.1763	383.0159	1.2457	5.9481		R ²	0.9989
0.2009	384.3727	1.0653	5.9516	4.3747	R	0.9995
0.2253	385.5286	0.9185	5.9546	4.5317	W _o	393.5708 cc/g (N ₂ gas)
0.2500	386.6146	0.7948	5.9574	4.6899	W _o (ads)	0.6088 cc/g (N ₂ ads)
0.2748	387.5707	0.6900	5.9599	4.8490	E _o	20.2843 kJ/mol
0.2999	388.4079	0.5998	5.9621	5.0116	x	0.5916 nm
0.3485	389.7796	0.4595	5.9656	5.3335	H-J equation results	
0.3985	390.9755	0.3501	5.9686	5.6804		
0.4240	391.4874	0.3045	5.9700	5.8655	slope	3.4388 cc/gA
0.4491	391.9963	0.2650	5.9713	6.0544	intersept	370.6454 cc/g (N ₂ gas)
0.4744	392.5223	0.2300	5.9726	6.2525	R ²	0.9538
0.4986	392.9232	0.2003	5.9736	6.4503	R	0.9766
0.5235	393.3301			6.6634	W _o	370.6454 cc/g (N ₂ gas)
0.5484	393.7274			6.8876	W _o (ads)	0.5733 cc/g (N ₂ ads)
0.5736	394.1174			7.1274	Single Point	
0.9490	398.0175					
					W _o (ads)	0.6157 cc/g (N ₂ ads)

Table A. 3. Micropore volume calculations from N₂ adsorption onto ACC-20, 12 hours heating

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)	
0.0010	296.9070	19.7340	5.6934		K
0.0052	324.4502	11.4383	5.7821		β
0.0081	334.4142	9.5917	5.8124		T
0.0100	339.3551	8.7707	5.8270		R
0.0303	366.5945	5.0563	5.9043		n
0.0506	378.2935	3.6820	5.9357		C(ads/gas)
0.0809	386.7069	2.6149	5.9577		
0.1024	389.9359	2.1477	5.9660		
0.1304	392.9947	1.7163	5.9738		
0.1521	394.7607	1.4667	5.9783		
0.1769	396.4423	1.2409	5.9825		
0.2000	397.7890	1.0712	5.9859	4.3688	
0.2250	399.0179	0.9202	5.9890	4.5298	
0.2496	400.1014	0.7966	5.9917	4.6873	
0.2746	401.0534	0.6908	5.9941	4.8478	
0.2994	401.9184	0.6015	5.9962	5.0083	
0.3479	403.3773	0.4610	5.9999	5.3295	
0.3978	404.6512	0.3514	6.0030	5.6754	
0.4233	405.2153	0.3056	6.0044	5.8604	
0.4485	405.7219	0.2659	6.0057	6.0498	
0.4733	406.2805	0.2314	6.0070	6.2437	
0.4987	406.6892	0.2002	6.0080	6.4511	
0.5234	407.1017			6.6625	
0.5485	407.5718			6.8886	
0.5735	407.9422			7.1265	
0.9487	412.0934				
					Single Point
				W ₀ (ads)	0.6374 cc/g (N ₂ ads)

Table A .4. Micropore volume calculations from N₂ adsorption onto ACC-20, baseline benzene sample

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)	K	12.0000 kJ-nm/g-mole
0.0029	293.5053	14.1195	5.6819		β	0.3400
0.0054	310.2515	11.2748	5.7374		T	77.3500 ° K
0.0086	322.1501	9.3546	5.7750		R	0.0083 kJ/g-mole-K
0.0099	325.8454	8.8090	5.7864		n	2.0000
0.0317	355.4565	4.9265	5.8734		C(ads/gas)	646.4962
0.0507	366.3762	3.6771	5.9037		D-R equation results	
0.0803	374.6712	2.6304	5.9260			
0.1025	378.1296	2.1459	5.9352			
0.1306	381.1726	1.7137	5.9433			
0.1526	383.0772	1.4616	5.9482			
0.1771	384.6884	1.2392	5.9524		slope	-0.0216 (kJ/mol) ²
0.2005	386.0285	1.0679	5.9559	4.3721	intersept	5.9807 (kJ/mol) ²
0.225	387.2596	0.9202	5.9591	4.5298	R ²	0.9993
0.2497	388.3639	0.7962	5.9619	4.6879	R	0.9996
0.2747	389.363	0.6904	5.9645	4.8484	W ₀	395.7239 cc/g (N ₂ gas)
0.2998	390.251	0.6001	5.9668	5.011	W ₀ (ads)	0.6121 cc/g (N ₂ ads)
0.351	391.8636	0.4533	5.9709	5.3505	E ₀	20.0322 kJ/mol
0.3983	393.0618	0.3505	5.9740	5.6790	x	0.5990 nm
0.4233	393.7086	0.3056	5.9756	5.8604	H-J equation results	
0.449	394.2352	0.2652	5.9769	6.0536		
0.4822	394.9005	0.2200	5.9786	6.3153		
0.4998	395.201	0.1989	5.9794	6.4603		
0.5232	395.6764			6.6608		
0.5486	396.0557			6.8895	W ₀	371.3165 cc/g (N ₂ gas)
0.5817	396.6292			7.2076	W ₀ (ads)	0.5744 cc/g (N ₂ ads)
0.9491	400.9805				Single Point	
					W ₀ (ads)	0.6202 cc/g (N ₂ ads)

Table A .5. Micropore volume calculations from N ₂ adsorption onto ACC-20, 10 cycle benzene sample						
P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)		
0.0015	296.3017	17.4853	5.6914		K	12.0000 kJ-nm/g-mole
0.0049	334.62	11.6983	5.8130		β	0.3400
0.0079	347.4861	9.6915	5.8507		T	77.3500 ° K
0.0098	352.847	8.8478	5.8660		R	0.0083 kJ/g-mole-K
0.0298	382.5004	5.1046	5.9467		n	2.0000
0.0493	394.4688	3.7465	5.9775		C(ads/gas)	646.4962
0.0795	403.2012	2.6514	5.9994		D-R equation results	
0.1044	407.0459	2.1114	6.0089		slope	-0.0204 (kJ/mol) ²
0.1275	409.5736	1.7544	6.0151		intersept	6.0497 (kJ/mol) ²
0.153	411.6284	1.4575	6.0201		R ²	0.9996
0.1767	413.135	1.2425	6.0238		R	0.9998
0.201	414.4763	1.0646	6.0270	4.3753	W ₀	423.9777 cc/g (N ₂ gas)
0.2254	415.5517	0.9180	6.0296	4.5323	W ₀ (ads)	0.6558 cc/g (N ₂ ads)
0.2503	416.5501	0.7934	6.0320	4.6918	E ₀	20.5829 kJ/mol
0.2749	417.4245	0.6896	6.0341	4.8497	x	0.5830 nm
0.2999	418.2288	0.5998	6.0360	5.0116	H-J equation results	
0.3485	419.5064	0.4595	6.0391	5.3335	slope	3.0757 cc/gA
0.3983	420.5877	0.3505	6.0417	5.6790	intersept	402.3151 cc/g (N ₂ gas)
0.4238	421.089	0.3048	6.0428	5.8640	R ²	0.9399
0.449	421.5661	0.2652	6.0440	6.0536	R	0.9695
0.4741	421.9328	0.2304	6.0448	6.2501	W ₀	402.3151 cc/g (N ₂ gas)
0.4987	422.2898	0.2002	6.0457	6.4511	W ₀ (ads)	0.6223 cc/g (N ₂ ads)
0.524	422.5773			6.6678	Single Point	
0.5488	422.8762			6.8913	W ₀ (ads)	0.6587 cc/g (N ₂ ads)
0.5739	423.1349			7.1304		
0.9498	425.8688					

Table A. 6. Micropore volume calculations from N₂ adsorption onto ACC-20, 20 cycle benzene sample

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t(Angstrom)	K	12.0000 kJ-nm/g-mole
0.0019	314.165	16.2371	5.7499		β	0.3400
0.005	339.0513	11.6096	5.8262		T	77.3500 ° K
0.0079	350.2253	9.6915	5.8586		R	0.0083 kJ/g-mole-K
0.0102	356.482	8.6954	5.8763		n	2.0000
0.0306	384.7122	5.0279	5.9525		C(ads/gas)	646.4962
0.0507	396.4112	3.6771	5.9825		D-R equation results	
0.0812	404.8499	2.6072	6.0035			
0.1022	408.0977	2.1514	6.0115			
0.1304	411.1798	1.7163	6.0190			
0.1522	412.9701	1.4657	6.0234		slope	-0.0193 (kJ/mol) ²
0.1768	414.571	1.2417	6.0272		intersept	6.0521 (kJ/mol) ²
0.2002	415.9024	1.0699	6.0305	4.3701	R ²	0.9982
0.2247	417.154	0.9218	6.0335	4.5278	R	0.9991
0.2494	418.2605	0.7975	6.0361	4.6860	W ₀	425.0156 cc/g (N ₂ gas)
0.2745	419.2226	0.6912	6.0384	4.8471	W ₀ (ads)	0.6574 cc/g (N ₂ ads)
0.2993	420.1485	0.6018	6.0406	5.0076	E ₀	21.1912 kJ/mol
0.348	421.5276	0.4608	6.0439	5.3302	x	0.5663 nm
0.3976	422.6813	0.3518	6.0466	5.6740	H-J equation results	
0.4231	423.1939	0.3060	6.0478	5.8589	slope	3.3722 cc/gA
0.4482	423.6812	0.2663	6.0490	6.0475	intersept	402.6539 cc/g (N ₂ gas)
0.4737	424.0618	0.2309	6.0499	6.2469	R ²	0.9406
0.498	424.6143	0.2010	6.0512	6.4453	R	0.9698
0.5241	424.8816			6.6687	W ₀	402.6539 cc/g (N ₂ gas)
0.5556	425.2709			6.9547	W ₀ (ads)	0.6228 cc/g (N ₂ ads)
0.5734	425.6227			7.1255	Single Point	
0.9497	428.9682				W ₀ (ads)	0.6635 cc/g (N ₂ ads)

Table A.7. Micropore volume calculations from N₂ adsorption onto ACC-20, 30 cycle benzene sample

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)	
0.0022	284.4991	15.4862	5.6507		K 12.0000 kJ-nm/g-mole
0.0049	307.1638	11.6983	5.7274		β 0.3400
0.0078	319.4427	9.7426	5.7666		T 77.3500 ° K
0.0102	325.8936	8.6954	5.7866		R 0.0083 kJ/g-mole-K
0.0296	353.841	5.1241	5.8688		n 2.0000
0.0493	365.8821	3.7465	5.9023		C(ads/gas) 646.4962
0.0795	374.6696	2.6514	5.9260		
0.1033	378.4284	2.1313	5.9360		D-R equation results
0.1268	381.0627	1.7638	5.9430		slope -0.0215 (kJ/mol) ²
0.1525	383.1676	1.4626	5.9485		intercept 5.9797 (kJ/mol) ²
0.1762	384.7342	1.2465	5.9526		R ² 0.9994
0.2006	386.0447	1.0673	5.9560	4.3727	R 0.9997
0.225	387.2028	0.9202	5.9589	4.5298	W ₀ 395.3314 cc/g (N ₂ gas)
0.2498	388.183	0.7957	5.9615	4.6886	W ₀ (ads) 0.6115 cc/g (N ₂ ads)
0.2747	389.0768	0.6904	5.9638	4.8484	E ₀ 20.0442 kJ/mol
0.2995	389.8385	0.6011	5.9657	5.0089	x 0.5987 nm
0.3483	391.1623	0.4600	5.9691	5.3322	
0.3981	392.2688	0.3508	5.9719	5.6775	H-J equation results
0.4233	392.7859	0.3056	5.9733	5.8604	slope 3.1657 cc/gA
0.4485	393.1955	0.2659	5.9743	6.0498	intercept 373.5034 cc/g (N ₂ gas)
0.4732	393.5594	0.2315	5.9752	6.2429	R ² 0.9480
0.4983	393.9847	0.2007	5.9763	6.4478	R 0.9736
0.5234	394.3913			6.6625	W ₀ 373.5034 cc/g (N ₂ gas)
0.5483	394.7196			6.8867	W ₀ (ads) 0.5777 cc/g (N ₂ ads)
0.5732	395.0412			7.1235	
0.9488	397.5488				Single Point
					W ₀ (ads) 0.6149 cc/g (N ₂ ads)

Table A .8. Micropore volume calculations from N₂ adsorption onto ACC-20, 50 cycle benzene sample

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)	
0.0014	293.3918	17.8583	5.6815		K
0.0052	322.0066	11.4383	5.7746		β
0.0081	332.629	9.5917	5.8070		T
0.0099	337.1903	8.8090	5.8206		R
0.0303	365.3358	5.0563	5.9008		n
0.0496	376.4741	3.7314	5.9308		C(ads/gas)
0.0802	385.004	2.6330	5.9533		
0.1036	388.5827	2.1258	5.9625		
0.1269	391.0577	1.7624	5.9689		
0.1522	393.1372	1.4657	5.9742		
0.1758	394.7336	1.2498	5.9782		
0.2006	396.0985	1.0673	5.9817	4.3727	
0.225	397.2262	0.9202	5.9845	4.5298	
0.2498	398.2725	0.7957	5.9871	4.6886	
0.2746	399.1334	0.6908	5.9893	4.8478	
0.2994	399.9696	0.6015	5.9914	5.0083	
0.348	401.3376	0.4608	5.9948	5.3302	
0.3979	402.4966	0.3512	5.9977	5.6761	
0.4235	402.9621	0.3053	5.9988	5.8618	
0.4484	403.4355	0.2661	6.0000	6.0490	
0.4735	403.9298	0.2311	6.0012	6.2453	
0.4986	404.3629	0.2003	6.0023	6.4503	
0.5234	404.725			6.6625	
0.5483	405.1101			6.8867	
0.5735	405.4115			7.1265	
0.9489	408.9989				

D-R equation results				
slope	-0.0191 (kJ/mol) ²			
intersept	6.0021 (kJ/mol) ²			
R ²	0.9945			
R	0.9973			
W ₀	404.2960 cc/g (N ₂ gas)			
W ₀ (ads)	0.6254 cc/g (N ₂ ads)			
E ₀	21.2960 kJ/mol			
x	0.5635 nm			

H-J equation results				
slope	3.3030 cc/gA			
intersept	382.9362 cc/g (N ₂ gas)			
R ²	0.9515			
R	0.9754			
W ₀	382.9362 cc/g (N ₂ gas)			
W ₀ (ads)	0.5923 cc/g (N ₂ ads)			
Single Point				
W ₀ (ads)	0.6326 cc/g (N ₂ ads)			

Table A .9. Micropore volume calculations from N₂ adsorption onto ACC-20, baseline acetone sample

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)	
0.0059	309.7176	10.8956	5.7357		K
0.0079	317.3193	9.6915	5.7599		β
0.0101	323.2725	8.7328	5.7785		T
0.0321	352.9846	4.8908	5.8664		R
0.051	363.7821	3.6626	5.8966		n
0.0813	372.0367	2.6047	5.9190		C(ads/g)
0.1027	375.3724	2.1422	5.9279		
0.1312	378.4274	1.7060	5.9360		
0.1531	380.229	1.4565	5.9408		
0.1777	381.8386	1.2344	5.9450		
0.2006	383.1553	1.0673	5.9484		
0.2255	384.35	0.9175	5.9516	4.5330	
0.2499	385.42	0.7952	5.9543	4.6892	
0.275	386.3459	0.6893	5.9567	4.8503	
0.2999	387.1705	0.5998	5.9589	5.0116	
0.3483	388.556	0.4600	5.9624	5.3322	
0.3983	389.7744	0.3505	5.9656	5.6790	
0.432	390.5662	0.2913	5.9676	5.9250	
0.4492	390.9103	0.2649	5.9685	6.0552	
0.4827	391.561	0.2194	5.9701	6.3194	
0.4996	391.8922	0.1992	5.9710	6.4587	
0.5245	392.3656	0.1722	5.9722	6.6722	
0.5487	392.7825			6.8904	
0.5735	393.1872			7.1265	
					D-R equation results
					slope
					-0.0220 (kJ/mol) ²
					intersept
					5.9736 (kJ/mol) ²
					R ²
					0.9994
					R
					0.9997
					W ₀
					392.9223 cc/g (N ₂ gas)
					W ₀ (ads)
					0.6078 cc/g (N ₂ ads)
					E ₀
					19.8343 kJ/mol
					x
					0.6050 nm
					H-J equation results
					slope
					3.3440 cc/gA
					intersept
					370.1742 cc/g (N ₂ gas)
					R ²
					0.9675
					R
					0.9836
					W ₀
					370.1742 cc/g (N ₂ gas)
					W ₀ (ads)
					0.5726 cc/g (N ₂ ads)
					Single Point
					W ₀ (ads)
					0.6140 cc/g (N ₂ ads)
0.9492	396.9561				

Table A .10. Micropore volume calculations from N₂ adsorption onto ACC-20, 10 cycle acetone sample

P/P _o	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)	K	12.0000 kJ-nm/g-mole
0.0021	285.6296	15.7225	5.6547		β	0.3400
0.0049	307.5003	11.6983	5.7285		T	77.3500 ° K
0.0079	319.3986	9.6915	5.7664		R	0.0083 kJ/g-mole-K
0.0098	324.7705	8.8478	5.7831		n	2.0000
0.0306	355.0817	5.0279	5.8723		C(ads/g)	646.4962
0.049	366.2679	3.7617	5.9034		D-R equation results	
0.0796	375.3073	2.6487	5.9277			
0.1039	379.1813	2.1204	5.9380		slope	-0.0214 (kJ/mol) ²
0.1273	381.7807	1.7571	5.9448		intersept	5.9807 (kJ/mol) ²
0.1531	383.8612	1.4565	5.9503		R ²	0.9985
0.1767	385.3345	1.2425	5.9541		R	0.9993
0.2011	386.702	1.0640	5.9577	4.3760	W _o	395.7171 cc/g (N ₂ gas)
0.2254	387.764	0.9180	5.9604	4.5323	W _o (ads)	0.6121 cc/g (N ₂ ads)
0.2503	388.7658	0.7934	5.9630	4.6918	E _o	20.1274 kJ/mol
0.2751	389.6628	0.6889	5.9653	4.8510	x	0.5962 nm
0.3001	390.4412	0.5991	5.9673	5.0129	H-J equation results	
0.3487	391.7033	0.4590	5.9705	5.3349		
0.3988	392.7459	0.3495	5.9732	5.6825	slope	2.9829 cc/gA
0.4241	393.2293	0.3043	5.9744	5.8663	intersept	374.9699 cc/g (N ₂ gas)
0.4493	393.6436	0.2647	5.9754	6.0560	R ²	0.9351
0.4739	393.9785	0.2306	5.9763	6.2485	R	0.9670
0.4987	394.2956	0.2002	5.9771	6.4511	W _o	374.9699 cc/g (N ₂ gas)
0.5238	394.6061			6.6660	W _o (ads)	0.5800 cc/g (N ₂ ads)
0.5489	394.8931			6.8923	Single Point	
0.5739	395.1563			7.1304		
0.9495	397.363				W _o (ads)	0.6146 cc/g (N ₂ ads)

Table A .11. Micropore volume calculations from N ₂ adsorption onto ACC-20, 20 cycle acetone sample						
P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)		
0.0028	285.8095	14.2896	5.6553		K	12.0000 kJ-nm/g-mole
0.005	301.5122	11.6096	5.7088		β	0.3400
0.008	314.467	9.6412	5.7509		T	77.3500 ° K
0.0099	320.6661	8.8090	5.7704		R	0.0083 kJ/g-mole-K
0.0335	351.4872	4.7701	5.8622		n	2.0000
0.05	360.6077	3.7115	5.8878		C(ads/g)	646.4962
0.08	369.1331	2.6382	5.9112		D-R equation results	
0.1038	372.8271	2.1222	5.9211		slope	-0.0220 (kJ/mol) ²
0.1271	375.3821	1.7597	5.9279		intersept	5.9659 (kJ/mol) ²
0.1536	377.4925	1.4515	5.9336		R ²	0.9996
0.1769	379.0497	1.2409	5.9377		R	0.9998
0.2007	380.4018	1.0666	5.9412	4.3734	W ₀	389.8929 cc/g (N ₂ gas)
0.225	381.562	0.9202	5.9443	4.5298	W ₀ (ads)	0.6031 cc/g (N ₂ ads)
0.25	382.5635	0.7948	5.9469	4.6899	E ₀	19.8448 kJ/mol
0.2748	383.4436	0.6900	5.9492	4.8490	x	0.6047 nm
0.2997	384.2554	0.6005	5.9513	5.0102	H-J equation results	
0.3483	385.6823	0.4600	5.9550	5.3322	slope	3.5176 cc/gA
0.3986	386.8272	0.3499	5.9580	5.6811	intersept	366.1503 cc/g (N ₂ gas)
0.4236	387.3307	0.3051	5.9593	5.8626	R ²	0.9598
0.449	387.8468	0.2652	5.9606	6.0536	R	0.9797
0.4741	388.2743	0.2304	5.9617	6.2501	W ₀	366.1503 cc/g (N ₂ gas)
0.499	388.7075	0.1998	5.9628	6.4536	W ₀ (ads)	0.5664 cc/g (N ₂ ads)
0.5243	389.1168			6.6704	Single Point	
0.5493	389.5006			6.8960	W ₀ (ads)	0.6084 cc/g (N ₂ ads)
0.5744	389.8263					
0.949	393.3257					

Table A .12. Micropore volume calculations from N₂ adsorption onto ACC-20, 30 cycle acetone sample

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)	
0.0019	283.3898	16.2371	5.6468		K
0.0049	308.2291	11.6983	5.7308		β
0.008	320.6945	9.6412	5.7705		T
0.0098	326.089	8.8478	5.7872		R
0.031	357.0866	4.9905	5.8780		n
0.0509	369.0362	3.6674	5.9109		C(ads/g)
0.0805	377.4717	2.6252	5.9335		
0.1025	381.0048	2.1459	5.9428		
0.1305	384.1593	1.7150	5.9511		
0.1529	386.0513	1.4585	5.9560		
0.1775	387.759	1.2360	5.9604		
0.2007	389.1232	1.0666	5.9639	4.3734	
0.2256	390.3569	0.9169	5.9671	4.5336	
0.2501	391.4387	0.7943	5.9698	4.6905	
0.2751	392.432	0.6889	5.9724	4.8510	
0.2999	393.3322	0.5998	5.9747	5.0116	
0.3485	394.7857	0.4595	5.9783	5.3335	
0.3982	396.1305	0.3506	5.9817	5.6783	
0.4237	396.7733	0.3050	5.9834	5.8633	
0.449	397.3339	0.2652	5.9848	6.0536	
0.474	397.8468	0.2305	5.9861	6.2493	
0.499	398.3563	0.1998	5.9873	6.4536	
0.5237	398.8278			6.6652	
0.5487	399.2301			6.8904	
0.5735	399.6756				
0.9492	396.9561				
					Single Point
					W ₀ (ads) 0.6140 cc/g (N ₂ ads)

D-R equation results

slope	-0.0217 (kJ/mol) ²
intersept	5.9883 (kJ/mol) ²
R ²	0.9983
R	0.9991
W ₀	398.7329 cc/g (N ₂ gas)
W ₀ (ads)	0.6168 cc/g (N ₂ ads)
E ₀	19.9463 kJ/mol
x	0.6016 nm

H-J equation results

slope	3.9457 cc/gA
intersept	373.0249 cc/g (N ₂ gas)
R ²	0.9655
R	0.9826
W ₀	373.0249 cc/g (N ₂ gas)
W ₀ (ads)	0.5770 cc/g (N ₂ ads)

Table A .13. Micropore volume calculations from N₂ adsorption onto ACC-20, 50 cycle acetone sample

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t(Angstrom)	
0.001	296.907	19.7340	5.6934		K 12.0000 kJ-nm/g-mole
0.0052	324.4502	11.4383	5.7821		β 0.3400
0.0081	334.4142	9.5917	5.8124		T 77.3500 ° K
0.01	339.3551	8.7707	5.8270		R 0.0083 kJ/g-mole-K
0.0303	366.5945	5.0563	5.9043		n 2.0000
0.0506	378.2935	3.6820	5.9357		C(ads/g) 646.4962
0.0809	386.7069	2.6149	5.9577		
0.1024	389.9359	2.1477	5.9660		
0.1304	392.9947	1.7163	5.9738		D-R equation results
0.1521	394.7607	1.4667	5.9783		slope -0.0176 (kJ/mol) ²
0.1769	396.4423	1.2409	5.9825		intersept 6.0039 (kJ/mol) ²
0.2	397.789	1.0712	5.9859	4.3688	R ² 0.9801
0.225	399.0179	0.9202	5.9890	4.5298	R 0.9900
0.2496	400.1014	0.7966	5.9917	4.6873	W ₀ 405.0225 cc/g (N ₂ gas)
0.2746	401.0534	0.6908	5.9941	4.8478	W ₀ (ads) 0.6265 cc/g (N ₂ ads)
0.2994	401.9184	0.6015	5.9962	5.0083	E ₀ 22.1919 kJ/mol
0.3479	403.3773	0.4610	5.9999	5.3295	x 0.5407 nm
0.3978	404.6512	0.3514	6.0030	5.6754	
0.4233	405.2153	0.3056	6.0044	5.8604	H-J equation results
0.4485	405.7219	0.2659	6.0057	6.0498	slope 3.7844 cc/gA
0.4733	406.2805	0.2314	6.0070	6.2437	intersept 382.4406 cc/g (N ₂ gas)
0.4987	406.6892	0.2002	6.0080	6.4511	R ² 0.9616
0.5234	407.1017			6.6625	R 0.9806
0.5485	407.5718			6.8886	W ₀ 382.4406 cc/g (N ₂ gas)
0.5735	407.9422				W ₀ (ads) 0.5916 cc/g (N ₂ ads)
0.9487	412.0934				Single Point
					W ₀ (ads) 0.6374 cc/g (N ₂ ads)

Table A .14. Micropore volume calculations from N₂ adsorption onto untreated ACC-20, QA test 1

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t (Angstrom)	
0.003	273.0971	13.9561	5.6098		K 12.0000 kJ-nm/g-mole
0.0051	286.2762	11.5230	5.6570		β 0.3400
0.008	296.4607	9.6412	5.6919		T 77.3500 ° K
0.01	301.7907	8.7707	5.7097		R 0.0083 kJ/g-mole-K
0.0314	327.1285	4.9537	5.7904		n 2.0000
0.0495	335.8676	3.7364	5.8167		C(ads/gas) 646.4962
0.0822	343.5775	2.5819	5.8394		
0.102	346.2742	2.1551	5.8472		D-R equation results
0.126	348.8352	1.7746	5.8546	3.8710	slope -0.0209 (kJ/mol) ²
0.1504	350.9134	1.4843	5.8605	4.0409	intersept 5.8962 (kJ/mol) ²
0.1755	352.7164	1.2523	5.8657	4.2089	R ² 0.9975
0.2001	354.2203	1.0706	5.8699	4.3695	R 0.9988
0.225	355.5901	0.9202	5.8738	4.5298	W ₀ 363.6711 cc/g (N ₂ gas)
0.2497	356.8617	0.7962	5.8773	4.6879	W ₀ (ads) 0.5625 cc/g (N ₂ ads)
0.2746	357.9971	0.6908	5.8805	4.8478	E ₀ 20.3276 kJ/mol
0.2996	358.9944	0.6008	5.8833	5.0096	x 0.5903 nm
0.3481	360.7807	0.4605	5.8883	5.3308	
0.3982	362.4851	0.3506	5.8930	5.6783	H-J equation results
0.4237	363.2137	0.3050	5.8950	5.8633	slope 4.7640 cc/gA
0.4486	363.8337	0.2658	5.8967	6.0506	intersept 334.6149 cc/g (N ₂ gas)
0.4734	364.5548	0.2313	5.8987	6.2445	R ² 0.9733
0.4988	365.1532	0.2001	5.9003	6.4520	R 0.9866
0.5233	365.8008			6.6617	W ₀ 334.6149 cc/g (N ₂ gas)
0.5485	366.442			6.8886	W ₀ (ads) 0.5176 cc/g (N ₂ ads)
0.5733	367.0093				
					Single Point
0.9491	374.4317				W ₀ (ads) 0.5792 cc/g (N ₂ ads)

Table A .15. Micropore volume calculations from N ₂ adsorption onto untreated ACC-20, QA test 2						
P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t(Angstrom)		
0.0017	278.8065	16.8186	5.6305		K	12.0000 kJ-nm/g-mole
0.0049	299.0854	11.6983	5.7007		β	0.3400
0.0079	308.9667	9.6915	5.7332		T	77.3500 ° K
0.0098	313.6133	8.8478	5.7482		R	0.0083 kJ/g-mole-K
0.0334	339.5479	4.7785	5.8276		n	2.0000
0.0505	347.0493	3.6869	5.8495		C(ads/gas)	646.4962
0.0813	353.8719	2.6047	5.8689			
0.1016	356.5523	2.1625	5.8765		D-R equation results	
0.1294	359.1837	1.7293	5.8838		slope	-0.0179 (kJ/mol) ²
0.1510	360.8303	1.4780	5.8884		intersept	5.9164 (kJ/mol) ²
0.1762	362.3106	1.2465	5.8925		R ²	0.9959
0.2000	363.5621	1.0712	5.8960	4.3688	R	0.9979
0.2249	364.7033	0.9207	5.8991	4.5291	W ₀	371.0914 cc/g (N ₂ gas)
0.2498	365.6729	0.7957	5.9017	4.6886	W ₀ (ads)	0.5740 cc/g (N ₂ ads)
0.2748	366.5721	0.6900	5.9042	4.8490	E ₀	21.9553 kJ/mol
0.2995	367.3648	0.6011	5.9064	5.0089	x	0.5466 nm
0.3483	368.6247	0.4600	5.9098	5.3322	H-J equation results	
0.3982	369.7494	0.3506	5.9128	5.6783	slope	3.2322 cc/gA
0.4239	370.2744	0.3046	5.9142	5.8648	intersept	350.6766 cc/g (N ₂ gas)
0.4490	370.7654	0.2652	5.9156	6.0536	R ²	0.9550
0.4740	371.2127	0.2305	5.9168	6.2493	R	0.9773
0.4989	371.6354	0.2000	5.9179	6.4528	W ₀	370.6454 cc/g (N ₂ gas)
0.5237	372.0000			6.6652	W ₀ (ads)	0.5424 cc/g (N ₂ ads)
0.5484	372.3865			6.8876	Single Point	
0.5737	372.7413			7.1284		
0.9490	376.1484				W ₀ (ads)	0.5818 cc/g (N ₂ ads)

Table A .16. Micropore volume calculations from N₂ adsorption onto untreated ACC-20, QA test 3

P/P ₀	W (cc/g STP gas)	A ² (kJ/mol) ²	ln (W)	t(Angstrom)	K	12.0000 kJ-nm/g-mole
0.0017	249.8243	16.8186	5.5208		β	0.3400
0.0050	271.7249	11.6096	5.6048		T	77.3500 ° K
0.0082	281.7896	9.5429	5.6412		R	0.0083 kJ/g-mole-K
0.0098	285.5970	8.8478	5.6546		n	2.0000
0.0300	309.4900	5.0851	5.7349		C(ads/gas)	646.4962
0.0494	318.6287	3.7415	5.7640		D-R equation results	
0.0805	325.6343	2.6252	5.7858			
0.1032	328.4917	2.1331	5.7945			
0.1265	330.6142	1.7678	5.8010			
0.1513	332.3829	1.4749	5.8063			
0.1756	333.8188	1.2514	5.8106		slope	-0.0197 (kJ/mol) ²
0.2004	335.0253	1.0686	5.8142	4.3714	intersept	5.8378 (kJ/mol) ²
0.2250	336.9553	0.9202	5.8200	4.5298	R ²	0.9971
0.2499	337.7682	0.7952	5.8224	4.6892	R	0.9985
0.2747	338.5110	0.6904	5.8246	4.8484	W ₀	343.0183 cc/g (N ₂ gas)
0.2997	339.7413	0.6005	5.8282	5.0102	W ₀ (ads)	0.5306 cc/g (N ₂ ads)
0.3485	340.8325	0.4595	5.8314	5.3335	E ₀	20.9605 kJ/mol
0.3984	341.3165	0.3503	5.8328	5.6797	x	0.5725 nm
0.4240	341.7932	0.3045	5.8342	5.8655	H-J equation results	
0.4491	342.2440	0.2650	5.8355	6.0544		
0.4742	342.6073	0.2302	5.8378	6.2509		
0.5241	343.0177	0.1726	5.8388	6.6687		
0.5494	343.3539			6.8969		
0.5735	343.6810			7.1265		
					W ₀ (ads)	370.6454 cc/g (N ₂ gas)
					W ₀ (ads)	0.5025 cc/g (N ₂ ads)
					Single Point	
0.9487	394.0711					
					W ₀ (ads)	0.6095 cc/g (N ₂ ads)

Table A .17. BET surface area from N2 adsorption onto ACC-20, baseline heating

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0497	369.4262	1.4157E-04	slope	3.335E-03 g/cc N ₂ gas
0.0801	378.0094	2.3035E-04	intersept	-3.586E-05 g/cc N ₂ gas
0.1043	381.6808	3.0509E-04	R ²	0.9977
0.1274	384.1987	3.8001E-04	C	-91.9993
0.1531	386.327	4.6794E-04	V _M	303.1138 cc/g N ₂ gas
0.1771	387.9185	5.5479E-04	Surface Area	1319.3255 m ² /g
0.2013	389.337	6.4734E-04		

Constants

CSA of N ₂	16.2 angstrom ²
N _A	6.02214E+23 molecules/mole
Molar Vol	22414 cm ³ /mole

Table A .18. BET surface area from N2 adsorption onto ACC-20, 6 hours heating

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0492	364.3482	1.4202E-04	slope	3.374E-03 g/cc N ₂ gas
0.0799	373.065	2.3277E-04	intersept	-3.580E-05 g/cc N ₂ gas
0.1036	376.6842	3.0682E-04	R ²	0.9977
0.1269	379.2552	3.8324E-04	C	-93.2380
0.1525	381.382	4.7181E-04	V _M	299.5990 cc/g N ₂ gas
0.1763	383.0159	5.5881E-04	Surface Area	1304.0272 m ² /g
0.2009	384.3727	6.5407E-04		

Constants

CSA of N ₂	16.2 angstrom ²
N _A	6.02214E+23 molecules/mole
Molar Vol	22414 cm ³ /mole

Table A .19. BET surface area from N2 adsorption onto ACC-20, 12 hours heating

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0506	378.2935	1.4089E-04	slope	3.262E-03 g/cc N ₂ gas
0.0809	386.7069	2.2762E-04	intersept	-3.522E-05 g/cc N ₂ gas
0.1024	389.9359	2.9257E-04	R ²	0.9978
0.1304	392.9947	3.8157E-04	C	-91.6304
0.1521	394.7607	4.5441E-04	V _M	309.8821 cc/g N ₂ gas
0.1769	396.4423	5.4212E-04	Surface Area	1348.7849 m ² /g
0.2	397.789	6.2847E-04		

Constants

CSA of N ₂	16.2 angstrom ²
N _A	6.02214E+23 molecules/mole
Molar Vol	22414 cm ³ /mole

Table A .20. BET surface area from N2 adsorption onto ACC-20, baseline benzene

P/P ₀	W (cc/g STP gas)	1/[W(P ₀ /P - 1)]		
0.0507	366.3762	1.4577E-04	slope	3.361E-03 g/cc N ₂ gas
0.0803	374.6712	2.3303E-04	intersept	-3.595E-05 g/cc N ₂ gas
0.1025	378.1296	3.0203E-04	R ²	0.9978
0.1306	381.1726	3.9410E-04	C	-92.4933
0.1526	383.0772	4.7009E-04	V _M	300.7452 cc/g N ₂ gas
0.1771	384.6884	5.5945E-04	Surface Area	1309.0160 m ² /g
0.2005	386.0285	6.4965E-04		
Constants				
CSA of N ₂	16.2 angstrom ²			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .21. BET surface area from N2 adsorption onto ACC-20, 10 cycle benzene

P/P ₀	W (cc/g STP gas)	1/[W(P ₀ /P - 1)]		
0.0493	394.4688	1.3146E-04	slope	3.132E-03 g/cc N ₂ gas
0.0795	403.2012	2.1420E-04	intersept	-3.401E-05 g/cc N ₂ gas
0.1044	407.0459	2.8638E-04	R ²	0.9976
0.1275	409.5736	3.5679E-04	C	-91.0902
0.153	411.6284	4.3884E-04	V _M	322.7496 cc/g N ₂ gas
0.1767	413.135	5.1950E-04	Surface Area	1404.7917 m ² /g
0.201	414.4763	6.0695E-04		
Constants				
CSA of N ₂	16.2 angstrom ²			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .22. BET surface area from N2 adsorption onto ACC-20, 20 cycle benzene

P/P ₀	W (cc/g STP gas)	1/[W(P ₀ /P - 1)]		
0.0507	396.4112	1.3473E-04	slope	3.123E-03 g/cc N ₂ gas
0.0812	404.8499	2.1829E-04	intersept	-3.425E-05 g/cc N ₂ gas
0.1022	408.0977	2.7894E-04	R ²	0.9977
0.1304	411.1798	3.6469E-04	C	-90.1796
0.1522	412.9701	4.3471E-04	V _M	323.7546 cc/g N ₂ gas
0.1768	414.571	5.1806E-04	Surface Area	1409.1660 m ² /g
0.2002	415.9024	6.0185E-04		
Constants				
CSA of N ₂	16.2 angstrom ²			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .23. BET surface area from N2 adsorption onto ACC-20, 30 cycle benzene				
P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0493	365.8821	1.4173E-04	slope	3.357E-03 g/cc N ₂ gas
0.0795	374.6696	2.3051E-04	intersept	-3.554E-05 g/cc N ₂ gas
0.1033	378.4284	3.0442E-04	R ²	0.9976
0.1268	381.0627	3.8107E-04	C	-93.4657
0.1525	383.1676	4.6961E-04	V _M	301.0307 cc/g N ₂ gas
0.1762	384.7342	5.5593E-04	Surface Area	1310.2588 m ² /g
0.2006	386.0447	6.5002E-04		
Constants				
CSA of N ₂	16.2 angstrom ²			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .24. BET surface area from N2 adsorption onto ACC-20, 50 cycle benzene				
P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0496	376.4741	1.3862E-04	slope	3.276E-03 g/cc N ₂ gas
0.0802	385.004	2.2647E-04	intersept	-3.529E-05 g/cc N ₂ gas
0.1036	388.5827	2.9742E-04	R ²	0.9977
0.1269	391.0577	3.7167E-04	C	-91.8226
0.1522	393.1372	4.5664E-04	V _M	308.6057 cc/g N ₂ gas
0.1758	394.7336	5.4036E-04	Surface Area	1343.2294 m ² /g
0.2006	396.0985	6.3352E-04		
Constants				
CSA of N ₂	16.2 angstrom ²			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .25. BET surface area from N2 adsorption onto ACC-20, baseline acetone

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.051	363.7821	1.4773E-04	slope	3.389E-03 g/cc N ₂ gas
0.0813	372.0367	2.3787E-04	intersept	-3.655E-05 g/cc N ₂ gas
0.1027	375.3724	3.0491E-04	R ²	0.9978
0.1312	378.4274	3.9905E-04	C	-91.7121
0.1531	380.229	4.7544E-04	V _M	298.3127 cc/g N ₂ gas
0.1777	381.8386	5.6595E-04	Surface Area	1298.4285 m ² /g
0.2006	383.1553	6.5493E-04		
Constants				
CSA of N ₂	16.2 angstrom ²			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .26. BET surface area from N2 adsorption onto ACC-20, 10 cycle acetone

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.049	366.2679	1.4067E-04	slope	3.353E-03 g/cc N ₂ gas
0.0796	375.3073	2.3044E-04	intersept	-3.553E-05 g/cc N ₂ gas
0.1039	379.1813	3.0578E-04	R ²	0.9976
0.1273	381.7807	3.8208E-04	C	-93.3606
0.1531	383.8612	4.7094E-04	V _M	301.4286 cc/g N ₂ gas
0.1767	385.3345	5.5698E-04	Surface Area	1311.9907 m ² /g
0.2011	386.702	6.5094E-04		
Constants				
CSA of N ₂	16.2 angstrom ²			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .27. BET surface area from N2 adsorption onto ACC-20, 20 cycle acetone

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.05	360.6077	1.4595E-04	slope	3.410E-03 g/cc N ₂ gas
0.08	369.1331	2.3557E-04	intersept	-3.637E-05 g/cc N ₂ gas
0.1038	372.8271	3.1066E-04	R ²	0.9977
0.1271	375.3821	3.8789E-04	C	-92.7702
0.1536	377.4925	4.8074E-04	V _M	296.3761 cc/g N ₂ gas
0.1769	379.0497	5.6699E-04	Surface Area	1289.9992 m ² /g
0.2007	380.4018	6.6008E-04		
Constants				
CSA of N ₂	16.2 angstrom ²			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .28. BET surface area from N2 adsorption onto ACC-20, 30 cycle acetone

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0509	369.0362	1.4532E-04	slope	3.335E-03 g/cc N ₂ gas
0.0805	377.4717	2.3193E-04	intersept	-3.568E-05 g/cc N ₂ gas
0.1025	381.0048	2.9975E-04	R ²	0.9978
0.1305	384.1593	3.9069E-04	C	-92.4858
0.1529	386.0513	4.6755E-04	V _M	303.0595 cc/g N ₂ gas
0.1775	387.759	5.5655E-04	Surface Area	1319.0890 m ² /g
0.2007	389.1232	6.4528E-04		

Constants

CSA of N ₂	16.2 angstrom ²
N _A	6.02214E+23 molecules/mole
Molar Vol	22414 cm ³ /mole

Table A .29. BET surface area from N2 adsorption onto ACC-20, 50 cycle benzene

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0506	378.2935	1.4089E-04	slope	3.262E-03 g/cc N ₂ gas
0.0809	386.7069	2.2762E-04	intersept	-3.522E-05 g/cc N ₂ gas
0.1024	389.9359	2.9257E-04	R ²	0.9978
0.1304	392.9947	3.8157E-04	C	-91.6304
0.1521	394.7607	4.5441E-04	V _M	309.8821 cc/g N ₂ gas
0.1769	396.4423	5.4212E-04	Surface Area	1348.7849 m ² /g
0.2	397.789	6.2847E-04		

Constants

CSA of N ₂	16.2 angstrom ²
N _A	6.02214E+23 molecules/mole
Molar Vol	22414 cm ³ /mole

Table A .30. BET surface area from N2 adsorption onto untreated ACC-20, QA test 1

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0495	335.8676	1.5505E-04	slope	3.660E-03 g/cc N ₂ gas
0.0822	343.5775	2.6067E-04	intersept	-3.867E-05 g/cc N ₂ gas
0.102	346.2742	3.2802E-04	R ²	0.9978
0.126	348.8352	4.1327E-04	C	-93.6471
0.1504	350.9134	5.0447E-04	V _M	276.1216 cc/g N ₂ gas
0.1755	352.7164	6.0348E-04	Surface Area	1201.8398 m ² /g
0.2001	354.2203	7.0622E-04		
Constants				
CSA of N ₂	16.2 angstrom			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .31. BET surface area from N2 adsorption onto untreated ACC-20, QA test 2

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0505	347.0493	1.5325E-04	slope	3.573E-03 g/cc N ₂ gas
0.0813	353.8719	2.5008E-04	intersept	-3.923E-05 g/cc N ₂ gas
0.1016	356.5523	3.1718E-04	R ²	0.9978
0.1294	359.1837	4.1381E-04	C	-90.0738
0.1510	360.8303	4.9291E-04	V _M	282.9982 cc/g N ₂ gas
0.1762	362.3106	5.9034E-04	Surface Area	1231.7709 m ² /g
0.2000	363.5621	6.8764E-04		
Constants				
CSA of N ₂	16.2 angstrom			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			

Table A .32. BET surface area from N2 adsorption onto untreated ACC-20, QA test 3

P/P _o	W (cc/g STP gas)	1/[W(P _o /P - 1)]		
0.0494	318.6287	1.6310E-04	slope	3.873E-03 g/cc N ₂ gas
0.0805	325.6343	2.6885E-04	intersept	-4.167E-05 g/cc N ₂ gas
0.1032	328.4917	3.5032E-04	R ²	0.9977
0.1265	330.6142	4.3803E-04	C	-91.9240
0.1513	332.3829	5.3635E-04	V _M	261.0403 cc/g N ₂ gas
0.1756	333.8188	6.3808E-04	Surface Area	1136.1973 m ² /g
0.2004	335.0253	7.4808E-04		
Constants				
CSA of N ₂	16.2 angstrom			
N _A	6.02214E+23 molecules/mole			
Molar Vol	22414 cm ³ /mole			





DUDLEY KNOX LIBRARY



3 2768 00314248 0